

A Solution Accurate, Efficient and Stable Unsplit Staggered Mesh Scheme for Three Dimensional Magnetohydrodynamics

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Abstract

In this paper, we extend the unsplit staggered mesh scheme (USM) for 2D magnetohydrodynamics (MHD) [D. Lee, A. Deane, An Unsplit Staggered Mesh Scheme for Multidimensional Magnetohydrodynamics, *J. Comput. Phys.* 228 (2009) 952–975] to a full 3D MHD scheme. The scheme is a finite-volume Godunov method consisting of a constrained transport (CT) method and an efficient and accurate single-step, directionally unsplit multidimensional data reconstruction-evolution algorithm, which extends Colella’s original 2D corner transport upwind (CTU) method [P. Colella, Multidimensional Upwind Methods for Hyperbolic Conservation Laws, *J. Comput. Phys.* 87 (1990) 446–466]. We present two types of data reconstruction-evolution algorithms for 3D: (1) a reduced CTU scheme and (2) a full CTU scheme. The reduced 3D CTU scheme is a variant of a simple 3D extension of Colella’s 2D CTU method and is considered as a direct extension from the 2D USM scheme. The full 3D CTU scheme is our primary 3D solver which includes all multidimensional cross-derivative terms for stability. The latter method is logically analogous to the 3D unsplit CTU method by Saltzman [J. Saltzman, An unsplit 3D upwind method for hyperbolic conservation laws, *J. Comput. Phys.* 115 (1994) 153–168]. The major novelties in our algorithms are twofold. First, we extend the reduced CTU scheme to the full CTU scheme which is able to run with CFL numbers close to unity. Both methods utilize the transverse update technique developed in the 2D USM algorithm to account for transverse fluxes *without* solving intermediate Riemann problems, which in turn gives cost-effective 3D methods by reducing the total number of Riemann solves. The proposed algorithms are simple and efficient especially when including multidimensional MHD terms that maintain in-plane magnetic field dynamics. Second, we introduce a new CT scheme that makes use of proper upwind information in taking averages of electric fields. Our 3D USM schemes can be easily combined with various reconstruction methods (e.g., first-order Godunov, second-order MUSCL-Hancock, third-order PPM and fifth-order WENO), and a wide choice of 1D based Riemann solvers (e.g., local Lax-Friedrichs, HLLE, HLLC, HLLD, and Roe). The 3D USM-MHD solver is available in the University of Chicago Flash Center’s official FLASH release.

Key words: MHD; Magnetohydrodynamics; Constrained Transport; Corner Transport Upwind; Unsplit Scheme; Staggered Mesh; High-Order Godunov Method; Large CFL Number.

1. Introduction

Many astrophysical applications involve the study of magnetized flows generating shock waves. Modeling such flows requires numerical solution of the equations of magnetohydrodynamics (MHD) that couple the magnetic field to the gas hydrodynamics using Maxwell’s equations. A valid computer model needs to

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capture accurately the nonlinear shock propagation in the magnetized flows without sacrificing computational efficiency and stability.

Obviously, with suitable assumptions about flow symmetries, a simple approach to obtain a computationally efficient model is to solve a reduced system in 1D or 2D instead of 3D. However, a limitation of such reduced systems is that they cannot be used to understand complicated nonlinear physics occurring only in the full 3D situation. Although solving the reduced system can illustrate interesting characteristic features (e.g., the inverse energy cascade in 2D turbulence [39]), it is essential to use 3D simulations in order to understand the full nonlinear nature of MHD phenomena (e.g., the energy cascade from large scales to small scales in 3D turbulence).

There are two approaches in modeling multidimensional (i.e., 2D and 3D) algorithms for gas hydrodynamics and MHD in terms of spatial integration methods: split and unsplit. The directionally split method has the advantage of extending a 1D algorithm to higher dimensions, simply by conducting directional sweeps along additional dimensions, in which each sweep solves 1D sub-system. Thus, the Courant-Friedrichs-Lewy (CFL) numerical stability constraint of the split schemes in multi-dimensions is the same as the 1D constraint, which is to say $CFL \leq 1.0$. Despite their simplicity and robustness, however, a number of recent studies have revealed numerical problems in the split formulations of multidimensional MHD and gas hydrodynamics (e.g., loss of expected flow symmetries [2, 41], failure to preserve in-plane magnetic field evolution [30, 40], numerical artifacts due to a failure to compute proper strain rates on a grid scale [3]).

For MHD the use of an unsplit formulation is more critical than for hydrodynamics. This is because the split formulations fail to evolve the normal (in the sweep direction) magnetic field [18, 30, 31, 59]. For 2D MHD, Gardiner and Stone [30] identified the importance of such multidimensional consideration in their unsplit MHD scheme based on the corner transport upwind (CTU) [16] and the constrained transport (CT) [26] methods. Later, the authors proposed a 3D unsplit version of an unsplit MHD scheme in [31], in which the extension of the multidimensional MHD terms from their 2D algorithm to 3D is accomplished at the cost of considerable algorithmic complexity and a reduced stability limit ($CFL < 0.5$) in their 6-solve CTU+CT algorithm. It is known in a CTU-type 3D unsplit formulation that the full CFL stability limit (i.e., CFL number ≤ 1.0) can be recovered by accounting for intermediate Riemann problems fully, requiring 12 Riemann solves per zone per time step [55]. In general, the calculations associated with the Riemann solves are computationally expensive. Gardiner and Stone [31] considered two alternative options, an expensive 12-Riemann solve yielding the full CFL limit and a reduced 6-Riemann solve with a more constraining CFL condition (CFL number < 0.5). They found that the two approaches are similar in terms of computational cost and there is no significant difference in performance between them. The 6-solve scheme is chosen to be their primary 3D integrator because of its relatively low complexity in incorporating the multidimensional MHD terms.

The CTU formulation has an advantage in its compact design of one-step temporal update which is well-suited for multidimensional problems. However, it is limited to second-order. There has been much progress in other types of temporal update strategies that are higher than second-order accurate, taking a different path from CTU. Early attempts have utilized a Runge-Kutta (RK) based temporal update formulation coupled with spatially high-order reconstruction schemes in the finite-difference framework [6, 13, 35, 38, 44, 57, 58, 60]. Such RK-based high-order schemes have been also developed in the finite-volume framework [8, 22, 23, 37, 69] which has superior properties to that of finite-difference for resolving compressible flows on both uniform and AMR grids. The high-order RK temporal update strategies rely on multi-stage updates which add to the computational cost. Therefore it is desirable to retain a CTU-like one-step formulation, while retaining higher than second order accuracy. Recent work has been found to provide such efficiency using a new formulation so-called the Arbitrary Derivative Riemann Problem (ADER), see [9, 12, 24, 25, 61, 62, 64]. For solving multidimensional conservation laws, there has been another line of progress that tries to build genuinely multidimensional Riemann solvers for hydrodynamics

[1, 15, 27, 28, 32, 67]. Recently, a family of two-dimensional HLL-type Riemann solvers, HLLE [10] and HLLC [11], have been introduced and generalized by Balsara for both hydrodynamics and MHD. As shown in his work the multidimensional Riemann solvers are genuinely derived for 2D. A major improvement in MHD flows is that they inherently provide proper amount of numerical dissipation that is necessary to propagate magnetic fields in a stable manner. Alternatively, 1D Riemann solver formulations such as [30, 45] need to add extra dissipation for a stable upwinding. The use of multidimensional Riemann solvers is also shown to capture isotropic wave propagations better than the usual 1D approach. Furthermore, both types of solvers have been extended to 3D using a one-step predictor-corrector formulation.

The above mentioned strategies using high-order schemes and genuinely multidimensional Riemann solvers, provide improved solution accuracy and stability over CTU-CT formulations. In this paper, however, we are primarily interested in constructing a scheme that can be built on the 1D Riemann solver framework in line with a CTU-type method. The latter is (arguably) most widely used in many Godunov-type modern codes [16, 30, 31, 40, 43, 45–47, 55]. This design also benefits us in extending our 2D USM-MHD algorithm [40] to 3D without any modifications of the Riemann solvers. This paper describes an approach that provides (i) an algorithmic extension from 2D to 3D of the USM scheme of Lee and Deane [40], and (ii) the full CFL stability bound in 3D *without* the expense of 12 Riemann solves per cell per time step, and (iii) a new upwind biased electric fields construction scheme for CT. We show that the present USM scheme achieves a numerically efficient and consistent MHD algorithm in 3D without introducing a greater amount of additional complexity, while maintaining the full CFL stability range.

The paper is organized as follows: Section 2 describes our new 3D unsplit, single-step data reconstruction-evolution USM algorithm which consists of two stages, i.e., normal predictor and transverse corrector. Section 2 is subdivided into several subsections. We begin in Section 2.1 our discussion of the 3D USM scheme by considering the governing equations of MHD and their linearized form. The second-order MUSCL-Hancock approach for calculating the normal predictor is described in Section 2.2. We introduce in Section 2.3 our two 3D CTU schemes to compute the transverse correctors, which are efficient and essential for obtaining the full CFL stability range. In the subsections therein, we construct Riemann states at cell interfaces, focusing on our new transverse correctors that do not require the solution of any Riemann problem. The Riemann state calculations are completed by evolving the normal magnetic fields by a half time step, about which we describe in Section 2.4. The final update of the cell-centered conservative variables is shown in Section 2.5, followed by a new 3D upwind-biased CT update of magnetic fields in Section 2.6. We summarize our step-by-step, point-to-point 3D CTU schemes in Section 3. In Section 4 we present numerical results of various test problems that demonstrate the qualitative and quantitative performance of our schemes. We conclude the paper with a discussion in Section 5.

2. The three-dimensional USM scheme for MHD

2.1. MHD Equations

We consider solving the equations of MHD in conservation form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} - \mathbf{B} \mathbf{B}) + \nabla p_{tot} = 0, \quad (2)$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{B} - \mathbf{B} \mathbf{u}) = 0, \quad (3)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (\mathbf{u} E + \mathbf{u} p_{tot} - \mathbf{B} \mathbf{B} \cdot \mathbf{u}) = 0. \quad (4)$$

The conservative variables include the plasma mass density ρ , momenta $\rho \mathbf{u}$, magnetic fields \mathbf{B} , and total energy density E . The rest are the thermal pressure $p = (\gamma - 1)(E - \frac{1}{2}\rho U^2 - B_p)$, the magnetic pressure $B_p = (B_x^2 + B_y^2 + B_z^2)/2$, and the sum of the two is the total pressure $p_{tot} = p + B_p$. The ratio of specific heats is denoted with γ as usual. The solenoidal constraint $\nabla \cdot \mathbf{B} = 0$ is implied in the induction equation.

We write the above equations in a matrix form in 3D

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = 0, \quad (5)$$

where \mathbf{U} contains the eight MHD conservative variables, and \mathbf{F} , \mathbf{G} , and \mathbf{H} represent the corresponding conservative fluxes in x , y and z directions. It is often convenient to cast the conservative form of Equation (5) into a quasi-linearized representation in terms of primitive variables, $\mathbf{V} = (\rho, u, v, w, B_x, B_y, B_z, p)^T$, in order to discretize the coupled system of MHD equations (1)-(4),

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{A}_x \frac{\partial \mathbf{V}}{\partial x} + \mathbf{A}_y \frac{\partial \mathbf{V}}{\partial y} + \mathbf{A}_z \frac{\partial \mathbf{V}}{\partial z} = 0. \quad (6)$$

The coefficient matrices \mathbf{A}_x , \mathbf{A}_y , and \mathbf{A}_z are given by

$$\mathbf{A}_x = \begin{pmatrix} u & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & u & 0 & 0 & -\frac{B_x}{\rho} & \frac{B_y}{\rho} & \frac{B_z}{\rho} & \frac{1}{\rho} \\ 0 & 0 & u & 0 & -\frac{B_y}{\rho} & -\frac{B_x}{\rho} & 0 & 0 \\ 0 & 0 & 0 & u & -\frac{B_z}{\rho} & 0 & -\frac{B_x}{\rho} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B_y & -B_x & 0 & -v & u & 0 & 0 \\ 0 & B_z & 0 & -B_x & -w & 0 & u & 0 \\ 0 & \gamma p & 0 & 0 & -k\mathbf{u} \cdot \mathbf{B} & 0 & 0 & u \end{pmatrix}, \quad (7)$$

$$\mathbf{A}_y = \begin{pmatrix} v & 0 & \rho & 0 & 0 & 0 & 0 & 0 \\ 0 & v & 0 & 0 & -\frac{B_y}{\rho} & -\frac{B_x}{\rho} & 0 & 0 \\ 0 & 0 & v & 0 & \frac{B_x}{\rho} & -\frac{B_y}{\rho} & \frac{B_z}{\rho} & \frac{1}{\rho} \\ 0 & 0 & 0 & v & 0 & -\frac{B_z}{\rho} & -\frac{B_y}{\rho} & 0 \\ 0 & -B_y & B_x & 0 & v & -u & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & B_z & -B_y & 0 & -w & v & 0 \\ 0 & 0 & \gamma p & 0 & 0 & -k\mathbf{u} \cdot \mathbf{B} & 0 & v \end{pmatrix}, \quad (8)$$

$$\mathbf{A}_z = \begin{pmatrix} w & 0 & 0 & \rho & 0 & 0 & 0 & 0 \\ 0 & w & 0 & 0 & -\frac{B_z}{\rho} & 0 & -\frac{B_x}{\rho} & 0 \\ 0 & 0 & w & 0 & 0 & -\frac{B_z}{\rho} & -\frac{B_y}{\rho} & 0 \\ 0 & 0 & 0 & w & \frac{B_x}{\rho} & \frac{B_y}{\rho} & -\frac{B_z}{\rho} & \frac{1}{\rho} \\ 0 & -B_z & 0 & B_x & w & 0 & -u & 0 \\ 0 & 0 & -B_z & B_y & 0 & w & -v & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma p & 0 & 0 & -k\mathbf{u} \cdot \mathbf{B} & w \end{pmatrix}, \quad (9)$$

with $k = 1 - \gamma$.

For exposition purposes in this paper, we illustrate our calculations using a spatially second-order MUSCL-Hancock (MH) piecewise-linear method (PLM) for the normal predictor. Other normal predictor algorithms (e.g., piecewise parabolic method (PPM [17]), essentially non-oscillatory (ENO [34]), weighted essentially non-oscillatory (WENO [38]), etc.) can be adopted as well to give different degrees of solution accuracy

in our algorithm. In fact, we have implemented various reconstruction schemes of MH, PPM and 5th order WENO in FLASH, and they are available in the official FLASH distribution [21, 29, 40, 41].

This brings us to write the system (6) to obtain second-order accurate discretizations at cell faces,

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2} = \mathbf{V}_{i,j,k}^n + \frac{1}{2}[\pm \mathbf{I} - \frac{\Delta t}{\Delta x} \mathbf{A}_x] \Delta_x^{tvd} \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta y} \mathbf{A}_y \Delta_y^{up} \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta z} \mathbf{A}_z \Delta_z^{up} \mathbf{V}_{i,j,k}^n, \quad (10)$$

$$\mathbf{V}_{i,j,k,N,S}^{n+1/2} = \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta x} \mathbf{A}_x \Delta_x^{up} \mathbf{V}_{i,j,k}^n + \frac{1}{2}[\pm \mathbf{I} - \frac{\Delta t}{\Delta y} \mathbf{A}_y] \Delta_y^{tvd} \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta z} \mathbf{A}_z \Delta_z^{up} \mathbf{V}_{i,j,k}^n, \quad (11)$$

$$\mathbf{V}_{i,j,k,T,B}^{n+1/2} = \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta x} \mathbf{A}_x \Delta_x^{up} \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{2\Delta y} \mathbf{A}_y \Delta_y^{up} \mathbf{V}_{i,j,k}^n + \frac{1}{2}[\pm \mathbf{I} - \frac{\Delta t}{\Delta z} \mathbf{A}_z] \Delta_z^{tvd} \mathbf{V}_{i,j,k}^n, \quad (12)$$

where the plus and minus signs correspond to directions of N, E, S, W, T and B respectively in a natural way, see Figure 1. Each \mathbf{A}_d matrix represents the coefficient matrix in the d -direction evaluated at $\mathbf{V}_{i,j,k}^n$. The undivided difference operators in each d -direction are denoted as Δ_d^{tvd} and Δ_d^{up} , and they are suitably chosen slope vectors of $\mathbf{V}_{i,j,k}^n$ in each cell (i, j, k) using TVD and upwind slope limiters, respectively.

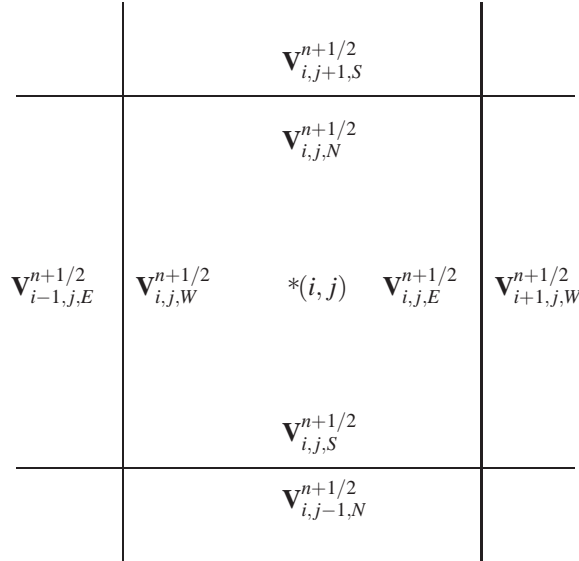


Fig. 1. The boundary extrapolated values on a 2D cell geometry. Our subscriptions N, S, E, W, T, B represent respectively north, south, east, west, top and bottom that are based on a reference point at the local cell center node (i, j, k) .

2.2. Normal Predictor

The first stage is to calculate the normal predictor states, including all the required multidimensional MHD terms (the MHD terms hereafter) [40] satisfying the solenoidal constraint $\nabla \cdot \mathbf{B} = 0$. We begin our discussion with the evolution of the normal field, B_N , which is treated separately from the other primitive variables. For instance, when $N = x$, we can define

$$\bar{\mathbf{V}}_x = \begin{bmatrix} \hat{\mathbf{V}}_x \\ B_x \end{bmatrix} \text{ and } \bar{\mathbf{A}}_x = \begin{bmatrix} \hat{\mathbf{A}}_x & \mathbf{A}_{B_x} \\ \mathbf{0} & 0 \end{bmatrix}. \quad (13)$$

Here $\hat{\mathbf{V}}_x$ is a 7×1 vector excluding B_x , $\hat{\mathbf{A}}_x$ is a 7×7 matrix omitting both the fifth row and column in the original matrix \mathbf{A}_x in Equation (7), and \mathbf{A}_{B_x} is a 7×1 vector,

$$\mathbf{A}_{B_x} = \left[0, -\frac{B_x}{\rho}, -\frac{B_y}{\rho}, -\frac{B_z}{\rho}, -v, -w, -k\mathbf{u} \cdot \mathbf{B} \right]^T. \quad (14)$$

Note that the hat (^) notation denotes the reduced system (i.e., the one corresponding to the usual 1D MHD equations) and the bar (-) notation indicates the re-assembled full system. Similarly for the other directions, we have

$$\bar{\mathbf{V}}_y = \begin{bmatrix} \hat{\mathbf{V}}_y \\ B_y \end{bmatrix}, \quad \bar{\mathbf{A}}_y = \begin{bmatrix} \hat{\mathbf{A}}_y & \mathbf{A}_{B_y} \\ \mathbf{0} & 0 \end{bmatrix}, \quad \mathbf{A}_{B_y} = \left[0, -\frac{B_x}{\rho}, -\frac{B_y}{\rho}, -\frac{B_z}{\rho}, -u, -w, -k\mathbf{u} \cdot \mathbf{B} \right]^T, \quad (15)$$

$$\bar{\mathbf{V}}_z = \begin{bmatrix} \hat{\mathbf{V}}_z \\ B_z \end{bmatrix}, \quad \bar{\mathbf{A}}_z = \begin{bmatrix} \hat{\mathbf{A}}_z & \mathbf{A}_{B_z} \\ \mathbf{0} & 0 \end{bmatrix}, \quad \mathbf{A}_{B_z} = \left[0, -\frac{B_x}{\rho}, -\frac{B_y}{\rho}, -\frac{B_z}{\rho}, -u, -v, -k\mathbf{u} \cdot \mathbf{B} \right]^T. \quad (16)$$

The term \mathbf{A}_{B_N} for each N will be our representation of the corresponding MHD term in this paper.

The first step of MH extrapolates $\mathbf{V}_{i,j,k}^n$ to construct the six multidimensional Riemann states $\mathbf{V}_{i,j,k,N,S,E,W,T,B}^{n+1/2}$ at cell interfaces to achieve second-order accuracy by using a total variation diminishing (TVD) slope limiter*. Although the slope limiter can be applied to either primitive or characteristic variables, we prefer the latter since it is less prone to generating spurious oscillations as noted in the literature [63, 66]. We do not apply any limiting to B_N , allowing the continuity of the normal field at cell faces (e.g., see discussion in [40]). To simplify our discussion, we focus on the x -direction in Equation (10). The others in Equations (11)-(12) can be computed in the similar way. We consider the first two terms in (10) that are related to the normal predictor

$$\begin{bmatrix} \hat{\mathbf{V}}_x \\ B_x \end{bmatrix}_{i,j,k,E,W}^{n+1/2,\parallel} = \begin{bmatrix} \hat{\mathbf{V}}_x \\ B_x \end{bmatrix}_{i,j,k}^n + \frac{1}{2} \left(\pm \begin{bmatrix} \hat{\mathbf{I}} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} - \frac{\Delta t}{\Delta x} \begin{bmatrix} \hat{\mathbf{A}}_x & \mathbf{A}_{B_x} \\ \mathbf{0} & 0 \end{bmatrix} \right)^n \Delta_x^{tvd} \bar{\mathbf{V}}_{i,j,k}^n, \quad (17)$$

where $\Delta_x^{tvd} \bar{\mathbf{V}}_{i,j,k}^n = \left(\Delta_x^{tvd} \hat{\mathbf{V}}_{i,j,k}^n, \Delta B_{x,i}^n \right)^T$ and $\Delta B_{x,i}^n = b_{x,i+1/2,j,k}^n - b_{x,i-1/2,j,k}^n$. The notations B_d and b_d denote cell-centered and cell face-centered magnetic fields respectively, with $d = x, y, z$. In CT, $\Delta B_{x,i}^n$ is constructed such that the numerical divergence is zero using the cell face-centered magnetic fields. In other words, $\Delta B_{x,i}^n$, $\Delta B_{y,j}^n$ and $\Delta B_{z,k}^n$ are chosen such that

$$\frac{\Delta B_{x,i}^n}{\Delta x} + \frac{\Delta B_{y,j}^n}{\Delta y} + \frac{\Delta B_{z,k}^n}{\Delta z} = 0, \quad (18)$$

where we analogously define $\Delta B_{y,j}^n$ and $\Delta B_{z,k}^n$. Solving a system in relation (17) is equivalent to considering two sub-systems

$$\begin{cases} \hat{\mathbf{V}}_{x,i,j,k,E,W}^{n+1/2,\parallel} = \hat{\mathbf{V}}_{x,i,j,k}^n + \frac{1}{2} \left(\pm \hat{\mathbf{I}} - \frac{\Delta t}{\Delta x} \hat{\mathbf{A}}_x \right)_{i,j,k}^n \Delta_x^{tvd} \hat{\mathbf{V}}_{i,j,k}^n - \frac{\Delta t}{2\Delta x} (\mathbf{A}_{B_x})_{i,j,k}^n \Delta B_{x,i}^n, \\ (B_x)_{i,j,k,E,W}^{n+1/2,\parallel} = B_{x,i,j,k}^n \pm \frac{1}{2} \Delta B_{x,i}^n. \end{cases} \quad (19)$$

The second relation in (19) is nothing but

$$(B_x)_{i,j,k,E,W}^{n+1/2,\parallel} = B_{x,i,j,k}^n \pm \frac{1}{2} \Delta B_{x,i}^n = b_{x,i\pm 1/2,j,k}^n, \quad (20)$$

* For instance, limiters such as minmod, van Leer's, monotonized central (MC), or a hybrid combination of them on different wave structures [7] can be used.

because we use a simple arithmetic averaging to obtain the cell-centered magnetic field using the divergence-free fields at cell interface centers,

$$B_{x,i,j,k}^n = \frac{1}{2} \left(b_{x,i+1/2,j,k}^n + b_{x,i-1/2,j,k}^n \right). \quad (21)$$

Applying the characteristic tracing method in x -normal direction in (19) yields

$$\hat{\mathbf{V}}_{x,i,j,k,W}^{n+1/2,\parallel} = \hat{\mathbf{V}}_{x,i,j,k}^n + \frac{1}{2} \sum_{m; \lambda_{x,i,j,k}^m < 0} \left(-1 - \frac{\Delta t}{\Delta x} \lambda_{x,i,j,k}^m \right) \mathbf{r}_{x,i,j,k}^m \Delta_x^{tvd} \hat{\alpha}_{i,j,k}^n - \frac{\Delta t}{2\Delta x} (\mathbf{A}_{B_x})_{i,j,k}^n \Delta B_{x,i}^n, \quad (22)$$

$$\hat{\mathbf{V}}_{x,i,j,k,E}^{n+1/2,\parallel} = \hat{\mathbf{V}}_{x,i,j,k}^n + \frac{1}{2} \sum_{m; \lambda_{x,i,j,k}^m > 0} \left(1 - \frac{\Delta t}{\Delta x} \lambda_{x,i,j,k}^m \right) \mathbf{r}_{x,i,j,k}^m \Delta_x^{tvd} \hat{\alpha}_{i,j,k}^n - \frac{\Delta t}{2\Delta x} (\mathbf{A}_{B_x})_{i,j,k}^n \Delta B_{x,i}^n. \quad (23)$$

A suitable TVD slope limiter along the x -normal direction is used in the undivided slope operator on each characteristic variable $\hat{\alpha}$

$$\Delta_x^{tvd} \hat{\alpha}_{i,j,k}^n = \text{TVD_Limiter} \left[\mathbf{l}_{x,i,j,k}^m \cdot (\hat{\mathbf{V}}_{x,i+1,j,k}^n - \hat{\mathbf{V}}_{x,i,j,k}^n), \mathbf{l}_{x,i,j,k}^m \cdot (\hat{\mathbf{V}}_{x,i,j,k}^n - \hat{\mathbf{V}}_{x,i-1,j,k}^n) \right]. \quad (24)$$

Here $\lambda_{x,i,j,k}^m$, $\mathbf{r}_{x,i,j,k}^m$, $\mathbf{l}_{x,i,j,k}^m$ represent respectively the eigenvalue, right and left eigenvectors of $\hat{\mathbf{A}}_x$, calculated at the corresponding cell center (i, j, k) in the x -direction at time step n . This completes the first part of our description on a single-step, data reconstruction-evolution algorithm in the x -normal direction.

2.3. Transverse Corrector in USM

2.3.1. Review of Computing Transverse Flux Gradients using Characteristic Tracing

The transverse corrector adds the gradients of transverse fluxes to the normal predictors. This transverse corrector step plays a crucial role for stability in CTU. Generally speaking, the degree of accuracy is affected by the normal predictor, whereas numerical stability is strongly determined by the transverse corrector [14].

In [40], Lee and Deane noted that the transverse flux gradients, responsible for the cross-derivative terms in CTU, which assure stability for flows advecting along diagonal corner directions, can be replaced by a simpler approach that is based on characteristic tracing alone. This removes the need to solve the intermediate Riemann problems. As a result, this approach requires only two Riemann solutions in 2D (not counting the extra two Riemann solves to update the divergence-free magnetic fields by CT), while preserving the full stability of the CTU scheme. We review a pointwise description of the transverse corrector in USM for a moment. Consider the y -transverse flux gradient (i.e., the third term in (10)) which supplies the corrector term to the x -normal predictor states. For any left ($\hat{\mathbf{V}}_{y,i,j,k}$) and right ($\hat{\mathbf{V}}_{y,i,j+,k}$) states at cell (i, j, k) along y -direction, the jump conditions across the individual m -th wave gives

$$\hat{\mathbf{A}}_{y,i,j,k} \hat{\mathbf{V}}_{y,i,j-,k} + \sum_{m=1}^{m_0-1} \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \Delta_y^{up} \hat{\alpha}_{i,j,k}^n = \hat{\mathbf{A}}_{y,i,j,k} \hat{\mathbf{V}}_{y,i,j+,k} - \sum_{m=m_0}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \Delta_y^{up} \hat{\alpha}_{i,j,k}^n. \quad (25)$$

Now recall that the property of conservation [42, 63] across discontinuities of the Roe matrix \mathbf{A} . It states that the Roe matrix ensures conservation across a discontinuity between the left (\mathbf{V}_l) and right (\mathbf{V}_r) states, given by $\mathbf{Flux}(\mathbf{V}_r) - \mathbf{Flux}(\mathbf{V}_l) = \mathbf{A}(\mathbf{V}_r - \mathbf{V}_l)$. Applying this relation to $\hat{\mathbf{A}}_{y,i,j,k}$, $\hat{\mathbf{V}}_{y,i,j-,k}$ and $\hat{\mathbf{V}}_{y,i,j+,k}$, and from (25), we obtain

$$\mathbf{G}_{i,j+1/2} - \mathbf{G}_{i,j-1/2} = \hat{\mathbf{A}}_{y,i,j,k} (\hat{\mathbf{V}}_{y,i,j+,k} - \hat{\mathbf{V}}_{y,i,j-,k}) = \sum_{m=1}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \Delta_y^{up} \hat{\alpha}_{i,j,k}^n. \quad (26)$$

The upwind slope limiter Δ_y^{up} is applied to each characteristic variable $\hat{\alpha}_{i,j,k}^n$ as

$$\Delta_y^{\text{up}} \hat{\mathbf{G}}_{i,j,k}^n \begin{cases} \mathbf{I}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j+1,k}^n - \hat{\mathbf{V}}_{i,j,k}^n) & \text{if } \lambda_{y,i,j,k}^m < 0 \\ \mathbf{I}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j,k}^n - \hat{\mathbf{V}}_{i,j-1,k}^n) & \text{if } \lambda_{y,i,j,k}^m > 0 \end{cases} \quad (27)$$

In Equation (26) we see that the sum over all wave contributions gives an effective upwinding of transverse flux gradients in y -direction. The advantage in this approach is that there is no need to solve the intermediate Riemann problems to add the transverse flux gradient correction terms to the spatially reconstructed, temporally evolved, normal predictor states in order to gain the upwind stability in the CTU formulation. Because we rely on using the eigensystem in Equation (26), one might suspect that this characteristic tracing approach could be as expensive as directly solving the associated Riemann problems at each interface, followed by taking the gradient of the computed transverse fluxes. However, this is not the case because we reuse the y - (or x -) directional eigensystems that were already calculated in the normal predictor step in the y - (or x -) direction. Thus there is no need to compute any additional eigenstructure for each transverse direction, which makes our scheme much more computationally efficient than the standard CTU method. A Fortran-like pseudo code illustrating the algorithm is as follows:

```
do j=jmin,jmax
  do i=imin,imax

    ! Compute normal predictor in x-direction, and
    ! store x-directional normal predictor states & eigensystems in arrays
    call dataReconstructNormalDirection(x_dir, x_normalPredictStates, sigmaSum_x)

    ! Compute normal predictor in y-direction, and
    ! store y-directional normal predictor states & eigensystems in arrays
    call dataReconstructNormalDirection(y_dir, y_normalPredictStates, sigmaSum_y)

    ! Transverse Correction to the x-normal predictor
    x_normalPredictStates = x_normalPredictStates - 0.5*dt/dy*sigmaSum_y

    ! Transverse Correction to the y-normal predictor
    y_normalPredictStates = y_normalPredictStates - 0.5*dt/dx*sigmaSum_x

  end do
end do
```

In the above, the terms `sigmaSum_x` and `sigmaSum_y` represent the summation of all wave contributions in the x - and y -directions, respectively, given in Equation (26). The rest of the terms are self-explanatory.

Our approach to approximate the transverse flux gradients, solely using the characteristic tracing, greatly simplifies the overall unsplit CTU algorithm by reducing the number of required Riemann solves. In gas hydrodynamics, the proposed algorithm requires a total of three Riemann solves to update the solution from n to $n+1$ without compromising solution stability and accuracy. It will be shown for MHD in Section 2.4 that three additional Riemann problems (yielding a total of six) are required to update the divergence-free, cell face-centered magnetic fields using the CT method. Another advantage in our approach, especially for MHD, is the relatively simple handling of multidimensional MHD terms. This is because our method of adding transverse flux gradients provides a single-step, directionally unsplit data reconstruction-evolution algorithm to calculate Riemann states at cell interfaces. It is therefore much simpler to enforce the balance

between flux gradients in all three directions associated with the MHD terms. As noted in [31], complications arise in the standard full 12-solve CTU scheme, in which the MHD term balance seems to be hard to achieve in a series of partial transverse flux gradient updates based on dimensional splitting.

2.3.2. Reduced 3D CTU Scheme in USM: Interface State Update from n to $n + 1/2$ Time Step

Our first simple algorithm using the transverse corrector technique in the previous section is analogous to the 6-solve CTU in [31]. This approach can be viewed as a straightforward 3D extension of the 2D CTU scheme [16], omitting all the third-order cross-derivative terms such as $\partial^3/\partial_x\partial_y\partial_z$, while including the second-order cross-derivative terms that are provided in the 2D CTU method. The resulting Riemann state calculations account for flow information along the edge directions, but do not fully account for flow information along the diagonal corner directions, yielding a formal stability limit of CFL number less than 0.5^\dagger . This simple approach, referred to as the reduced 3D CTU scheme, can be directly extended from the 2D CTU [40] by adding the third additional transverse flux correction in z . That is, the x -normal predictors in Equations (22)-(23) are further corrected by including the transverse flux contributions from y, z -directions using the characteristic tracing approach described in the previous section, see also [40]. For instance, in Equation (10) the transverse corrector step can be updated, first by accounting for the y -transverse flux correction,

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2,y} = \mathbf{V}_{i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \mathbf{A}_y(\mathbf{V}_{i,j,k}^n) \Delta_y^{up} \mathbf{V}_{i,j,k}^n, \quad (28)$$

followed by the z -transverse flux correction,

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2} = \mathbf{V}_{i,j,k,E,W}^{n+1/2,y} - \frac{\Delta t}{2\Delta z} \mathbf{A}_z(\mathbf{V}_{i,j,k}^n) \Delta_z^{up} \mathbf{V}_{i,j,k}^n. \quad (29)$$

In these transverse corrector steps, it is important to use the *upwind* biased slope limiter instead of any form of TVD limiters as reviewed in Section 2.3.1. Note that in the original 2D CTU scheme by Colella [16], using the upwind flux gradients in the transverse directions is the key mechanism that guarantees the full CFL stability bound. We establish the same upwind couplings by means of using the upwind slope limiter for our transverse corrector. Using a TVD slope limiter instead would result in a reduced stability limit for our algorithm (and we avoid using it). The two transverse correction terms in (28) and (29) are calculated as in Section 2.3.1, completing our description of the reduced 3D CTU scheme.

2.3.3. Full 3D CTU Scheme in USM: Interface State Update from n to $n + 1/2$ Time Step

To establish the full stability limit (CFL number less than 1 in 3D) as featured in the 12-solve CTU scheme of Saltzman [55], we need one more step to couple diagonally moving flow effects. This situation occurs when the conservative quantities are advected across the corners diagonally with components of the local velocity fields (u, v, w) being of comparable orders of magnitude. In USM, these couplings can be added to the interface states by performing intermediate state calculations at $n + \frac{1}{3}$. They involve extra evaluations of the coefficient matrices and the undivided upwind differences in (28) and (29) at

$$\mathbf{V}_{i,j,k}^{n+1/3,z} = \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{3\Delta z} (\mathbf{A}_z)_{i,j,k}^n \Delta_z^{up} \mathbf{V}_{i,j,k}^n, \quad (30)$$

and

$$\mathbf{V}_{i,j,k}^{n+1/3,y} = \mathbf{V}_{i,j,k}^n - \frac{\Delta t}{3\Delta y} (\mathbf{A}_y)_{i,j,k}^n \Delta_y^{up} \mathbf{V}_{i,j,k}^n. \quad (31)$$

[†] One can easily prove this stability bound numerically for a 3D scalar advection equation using a standard von Neuman Fourier analysis, assuming a single Fourier mode solution $q_{I,J,K}^n = e^{i(\xi I \Delta x + \eta J \Delta y + \zeta K \Delta z)}$ where $i = \sqrt{-1}$; I, J, K as the grid indices; and ξ, η, ζ the wave numbers in x, y, z -directions respectively.

More specifically, the transverse correctors in Equations (28) and (29) are replaced by

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2,y} = \mathbf{V}_{i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \mathbf{A}_y(\mathbf{V}_{i,j,k}^{n+1/3,z}) \Delta_y^{up} \mathbf{V}_{i,j,k}^{n+1/3,z}, \quad (32)$$

and

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2} = \mathbf{V}_{i,j,k,E,W}^{n+1/2,y} - \frac{\Delta t}{2\Delta z} \mathbf{A}_z(\mathbf{V}_{i,j,k}^{n+1/3,y}) \Delta_z^{up} \mathbf{V}_{i,j,k}^{n+1/3,y}. \quad (33)$$

Here we make one important observation. Note that the additional re-evaluations of the matrices \mathbf{A}_y and \mathbf{A}_z at the $n + \frac{1}{3}$ states $\mathbf{V}_{i,j,k}^{n+1/3,z}$ and $\mathbf{V}_{i,j,k}^{n+1/3,y}$ simply mean that the corresponding eigensystems for the characteristic tracing in the transverse directions need to be re-calculated, incurring the corresponding additional cost. Considering the full 3D interface state calculations in Equations (10)-(12), there are a total of six additional eigensystem evaluations required for the transverse correctors, which becomes as expensive as directly solving the corresponding Riemann problems, making our scheme expensive. Therefore an efficient alternative approach is required. Noticing

$$\frac{\Delta t}{3\Delta z} (\mathbf{A}_z)_{i,j,k}^n \Delta_z^{up} \mathbf{V}_{i,j,k}^n = \frac{\Delta t}{3} \frac{\partial \mathbf{H}}{\partial z} \bigg|_{\mathbf{V}_{i,j,k}^n}, \quad (34)$$

and using a Taylor expansion at $\mathbf{V}_{i,j,k}^n$, we consider

$$\mathbf{A}_y(\mathbf{V}_{i,j,k}^{n+1/3,z}) = \frac{\partial \mathbf{G}}{\partial \mathbf{V}} \bigg|_{\mathbf{V}_{i,j,k}^{n+1/3,z}} = \frac{\partial \mathbf{G}}{\partial \mathbf{V}} \bigg|_{\mathbf{V}_{i,j,k}^n} - \frac{\Delta t}{3} \frac{\partial \mathbf{H}}{\partial z} \bigg|_{\mathbf{V}_{i,j,k}^n} \frac{\partial^2 \mathbf{G}}{\partial \mathbf{V}^2} \bigg|_{\mathbf{V}_{i,j,k}^n} = \mathbf{A}_y(\mathbf{V}_{i,j,k}^n) + O(\Delta t). \quad (35)$$

Ignoring the Δt error term in the matrix evaluations in Equation (35), we can replace respectively $\mathbf{A}_y(\mathbf{V}_{i,j,k}^{n+1/3,z})$ and $\mathbf{A}_z(\mathbf{V}_{i,j,k}^{n+1/3,y})$ with $\mathbf{A}_y(\mathbf{V}_{i,j,k}^n)$ and $\mathbf{A}_z(\mathbf{V}_{i,j,k}^n)$ in Equations (32)-(33). However, it is essential to retain $\Delta_y^{up} \mathbf{V}_{i,j,k}^{n+1/3,z} = \left(\partial \mathbf{V} / \partial y \big|_{\mathbf{V}_{i,j,k}^{n+1/3,z}} \right) \Delta y$ and $\Delta_z^{up} \mathbf{V}_{i,j,k}^{n+1/3,y} = \left(\partial \mathbf{V} / \partial z \big|_{\mathbf{V}_{i,j,k}^{n+1/3,y}} \right) \Delta z$ to couple the diagonal upwind corner transport. We proceed this as follows. Ignoring the $O(\Delta t)$ term and keeping the first-order approximation in Equation (35) for the matrix evaluation, the transverse corrector in Equation (32) becomes

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2,y} = \mathbf{V}_{i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \mathbf{A}_y(\mathbf{V}_{i,j,k}^n) \Delta_y^{up} \mathbf{V}_{i,j,k}^{n+1/3,z} \quad (36)$$

Using our transverse corrector strategy, we get

$$\hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,y} = \hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \sum_{m=1}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \Delta_y^{up} \hat{\alpha}_{i,j,k}^{n+1/3,z} - \frac{\Delta t}{2\Delta y} (\mathbf{A}_{B_y})_{i,j,k}^n \Delta B_{y,j}^{n+1/3,z}, \quad (37)$$

where the upwinding slope applied to each characteristic variable $\hat{\alpha}$ is given by

$$\Delta_y^{up} \hat{\alpha}_{i,j,k}^{n+1/3,z} = \begin{cases} \mathbf{l}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j+1,k}^{n+1/3,z} - \hat{\mathbf{V}}_{i,j,k}^{n+1/3,z}) & \text{if } \lambda_{y,i,j,k}^m < 0 \\ \mathbf{l}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j,k}^{n+1/3,z} - \hat{\mathbf{V}}_{i,j-1,k}^{n+1/3,z}) & \text{if } \lambda_{y,i,j,k}^m > 0 \end{cases}. \quad (38)$$

Notice that the MHD term at $n + \frac{1}{3}$ can be written as

$$\Delta B_{y,j}^{n+1/3,z} = \Delta_y \left(B_{y,j}^n - \frac{\Delta t}{3\Delta z} [(\hat{\mathbf{A}}_z)_{i,j,k}^n \Delta_z^{up} \hat{\mathbf{V}}_{i,j,k}^n + (\mathbf{A}_{B_z})_{i,j,k}^n \Delta B_{z,k}^n] \cdot \mathbf{e}_{B_y} \right) = \Delta_y \left(B_{y,j}^n + O(\Delta t) \right), \quad (39)$$

where \mathbf{e}_{B_y} is a unit vector in B_y direction for contraction and the hat notation implies the omission of the B_z components. However, in order to choose $\Delta B_{y,j}^{n+1/3,z}$ to enforce the numerical divergence to be zero always (see Equation (18)), we further drop the Δt error term and only take

$$\Delta B_{y,j}^{n+1/3,z} = \Delta_y B_{y,j}^n = b_{y,j+1/2}^n - b_{y,j-1/2}^n, \quad (40)$$

where $b_{y,j\pm 1/2}^n$ are the cell face-centered, divergence-free magnetic fields in y-direction.

The upwind differences in relation (38) are given by (assuming uniform spacing in each direction everywhere),

$$\begin{aligned} & \hat{\mathbf{V}}_{i,j+1,k}^{n+1/3,z} - \hat{\mathbf{V}}_{i,j,k}^{n+1/3,z} \\ &= \hat{\mathbf{V}}_{i,j+1,k}^n - \hat{\mathbf{V}}_{i,j,k}^n - \frac{\Delta t}{3\Delta z} \left[(\hat{\mathbf{A}}_z)_{i,j+1,k}^n \Delta_z^{up} \hat{\mathbf{V}}_{i,j+1,k}^n + (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j+1,k} - (\hat{\mathbf{A}}_z)_{i,j,k}^n \Delta_z^{up} \hat{\mathbf{V}}_{i,j,k}^n - (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j,k} \right] \\ &= \hat{\mathbf{V}}_{i,j+1,k}^n - \hat{\mathbf{V}}_{i,j,k}^n - \frac{\Delta t}{3\Delta z} \left[\sum_{h=1}^7 \lambda_{z,i,j+1,k}^h \mathbf{r}_{z,i,j+1,k}^h \Delta_z^{up} \hat{\alpha}_{i,j+1,k}^n - \sum_{l=1}^7 \lambda_{z,i,j,k}^l \mathbf{r}_{z,i,j,k}^l \Delta_z^{up} \hat{\alpha}_{i,j,k}^n \right. \\ & \quad \left. + (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j+1,k} - (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j,k} \right], \end{aligned} \quad (41)$$

and

$$\begin{aligned} & \hat{\mathbf{V}}_{i,j,k}^{n+1/3,z} - \hat{\mathbf{V}}_{i,j-1,k}^{n+1/3,z} \\ &= \hat{\mathbf{V}}_{i,j,k}^n - \hat{\mathbf{V}}_{i,j-1,k}^n - \frac{\Delta t}{3\Delta z} \left[(\hat{\mathbf{A}}_z)_{i,j,k}^n \Delta_z^{up} \hat{\mathbf{V}}_{i,j,k}^n + (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j,k} - (\hat{\mathbf{A}}_z)_{i,j-1,k}^n \Delta_z^{up} \hat{\mathbf{V}}_{i,j-1,k}^n - (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j-1,k} \right] \\ &= \hat{\mathbf{V}}_{i,j,k}^n - \hat{\mathbf{V}}_{i,j-1,k}^n - \frac{\Delta t}{3\Delta z} \left[\sum_{h=1}^7 \lambda_{z,i,j,k}^h \mathbf{r}_{z,i,j,k}^h \Delta_z^{up} \hat{\alpha}_{i,j,k}^n - \sum_{l=1}^7 \lambda_{z,i,j-1,k}^l \mathbf{r}_{z,i,j-1,k}^l \Delta_z^{up} \hat{\alpha}_{i,j-1,k}^n \right. \\ & \quad \left. + (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j,k} - (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j-1,k} \right], \end{aligned} \quad (42)$$

In the case of $\lambda_{y,i,j,k}^m > 0$ for all m , using (42), Equation (37) becomes

$$\hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,y} = \hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \sum_{m=1}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \mathbf{l}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j,k}^{n+1/3,z} - \hat{\mathbf{V}}_{i,j-1,k}^{n+1/3,z}) - \frac{\Delta t}{2\Delta y} (\mathbf{A}_{B_y})_{i,j,k}^n \Delta B_{y,j}^n \quad (43)$$

$$= \hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,\parallel} - \frac{\Delta t}{2\Delta y} \sum_{m=1}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \mathbf{l}_{y,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j,k}^n - \hat{\mathbf{V}}_{i,j-1,k}^n) - \frac{\Delta t}{2\Delta y} (\mathbf{A}_{B_y})_{i,j,k}^n \Delta B_{y,j}^n \quad (44)$$

$$\begin{aligned} & + \frac{\Delta t^2}{6\Delta y \Delta z} \left(\sum_{m=1}^7 \lambda_{y,i,j,k}^m \mathbf{r}_{y,i,j,k}^m \mathbf{l}_{y,i,j,k}^m \cdot \left[\sum_{h=1}^7 \lambda_{z,i,j,k}^h \mathbf{r}_{z,i,j,k}^h \Delta_z^{up} \hat{\alpha}_{i,j,k}^n - \sum_{l=1}^7 \lambda_{z,i,j-1,k}^l \mathbf{r}_{z,i,j-1,k}^l \Delta_z^{up} \hat{\alpha}_{i,j-1,k}^n \right. \right. \\ & \quad \left. \left. + (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j,k} - (\mathbf{A}_{B_z}^n \Delta B_z^n)_{i,j-1,k} \right] \right). \end{aligned} \quad (45)$$

Note that the terms in relation (44) are what we already established in the reduced 3D CTU scheme. The terms in relation (45) are new correction terms for the full 3D CTU scheme that need to be added to the reduced 3D CTU interface states in relation (44).

Similarly, the final form of x-interface states $\mathbf{V}_{i,j,k,E,W}^{n+1/2}$ in Equation (33) is established by adding another correction term appearing in $\Delta_z^{up} \hat{\mathbf{V}}_{i,j,k}^{n+1/3,y}$, giving the result (assuming $\lambda_{z,i,j,k}^m > 0$ for all m)

$$\mathbf{V}_{i,j,k,E,W}^{n+1/2} = \hat{\mathbf{V}}_{y,i,j,k,E,W}^{n+1/2,y} - \frac{\Delta t}{2\Delta z} \sum_{m=1}^7 \lambda_{z,i,j,k}^m \mathbf{r}_{z,i,j,k}^m \mathbf{l}_{z,i,j,k}^m \cdot (\hat{\mathbf{V}}_{i,j,k}^n - \hat{\mathbf{V}}_{i,j,k-1}^n) - \frac{\Delta t}{2\Delta z} (\mathbf{A}_{B_z})_{i,j,k}^n \Delta B_{z,k}^n \quad (46)$$

$$\begin{aligned} & + \frac{\Delta t^2}{6\Delta z \Delta y} \left(\sum_{m=1}^7 \lambda_{z,i,j,k}^m \mathbf{r}_{z,i,j,k}^m \mathbf{l}_{z,i,j,k}^m \cdot \left[\sum_{h=1}^7 \lambda_{y,i,j,k}^h \mathbf{r}_{y,i,j,k}^h \Delta_y^{up} \hat{\alpha}_{i,j,k}^n - \sum_{l=1}^7 \lambda_{y,i,j,k-1}^l \mathbf{r}_{y,i,j,k-1}^l \Delta_y^{up} \hat{\alpha}_{i,j,k-1}^n \right. \right. \\ & \quad \left. \left. + (\mathbf{A}_{B_y}^n \Delta B_y^n)_{i,j,k} - (\mathbf{A}_{B_y}^n \Delta B_y^n)_{i,j,k-1} \right] \right). \end{aligned} \quad (47)$$

Likewise, the terms in relation (47) are the extra correction terms required for the full 3D CTU scheme. They must be added to the reduced CTU terms in relation (46).

It is worth pointing out at this stage that all of the eigensystems in the full 3D CTU correction terms are readily available as they have been calculated and stored in the normal predictor step in each x, y, z -direction described in Section 2.2. In the normal predictor step, one can store not only the eigensystems, but also the two summations inside the square brackets in relations (45) and (47) (see also the simple pseudo code in Section 2.3.1). The only extra calculations imposing additional computational costs are therefore the upwind differencings inside the square brackets and the dot products in relations (45) and (47), which are computationally much more efficient compared to the calculation requirements in the 12-solve CTU scheme. This completes our description of the single-step, data reconstruction-evolution algorithm for all variables *except* the divergence-free normal magnetic fields at each cell face. The reconstructed interface states are second-order accurate in space and evolved to $n + \frac{1}{2}$ time step at each interface. The next step is to advance the remaining normal fields at the cell faces, finalizing the Riemann state calculations.

2.4. Advancing the Normal Fields from n to $n + 1/2$ Time Step using CT

In updating the normal fields to $n + \frac{1}{2}$, it is important to meet two conditions. The first is a continuity restriction of the normal magnetic field across cell interfaces [7, 18, 30, 40, 51]. The second is the divergence-free constraint of the normal fields on a computational grid. As a last step of our Riemann state calculations, we must evolve the normal field components at each cell boundary by a half time step, while satisfying the two conditions. We therefore follow the CT approach using the high-order Godunov fluxes that are solutions to a Riemann problem using the Riemann states $\mathbf{V}_{i,j,N,S,E,W,T,B}^{n+1/2}$ described in Sections 2.3.2 and 2.3.3. Our approach here is the 3D extension of the 2D method in using the same approach as in [40]. Here we briefly describe the procedure only in x -direction, which can be similarly applied to the other directions. We first solve Riemann problem at x interfaces as

$$\tilde{\mathbf{F}}_{i-1/2,j,k}^{*,n+1/2} = \text{RP} \left(\mathbf{V}_{i-1,j,k,E}^{n+1/2}, \mathbf{V}_{i,j,k,W}^{n+1/2} \right), \quad \tilde{\mathbf{F}}_{i+1/2,j,k}^{*,n+1/2} = \text{RP} \left(\mathbf{V}_{i,j,k,E}^{n+1/2}, \mathbf{V}_{i+1,j,k,W}^{n+1/2} \right), \quad (48)$$

With these high-order Godunov fluxes at the half time step we evolve the normal fields by a half time step using the CT update

$$b_{x,i+1/2,j,k}^{n+1/2} = b_{x,i+1/2,j,k}^n - \frac{\Delta t}{2\Delta y} \left\{ \tilde{E}_{z,i+1/2,j+1/2,k}^{*,n+1/2} - \tilde{E}_{z,i+1/2,j-1/2,k}^{*,n+1/2} \right\} - \frac{\Delta t}{2\Delta z} \left\{ -\tilde{E}_{y,i+1/2,j,k+1/2}^{*,n+1/2} + \tilde{E}_{y,i+1/2,j,k-1/2}^{*,n+1/2} \right\}, \quad (49)$$

where the duality relationship between the electric fields and the high-order Godunov fluxes [5] is assumed in the expression. The electric fields $\tilde{E}_z^{*,n+1/2}$ in (49) can be constructed based on the MEC method [40] that takes an arithmetic average of four Taylor series expansions of the fluxes given by (48) to obtain them (e.g., see Equation (53) in Section 2.6.1). The normal fields in (49) satisfy the divergence-free constraint as well as the continuity restriction across cell interfaces as they are direct solutions to numerical induction equations via the CT approach.

Given these updated cell face-centered divergence-free fields, the Riemann states at x -interfaces are updated as

$$\mathbf{V}_{i,j,k,E}^{n+1/2} \cdot \mathbf{e}_{B_x} = b_{x,i+1/2,j,k}^{n+1/2}, \quad \mathbf{V}_{i,j,k,W}^{n+1/2} \cdot \mathbf{e}_{B_x} = b_{x,i-1/2,j,k}^{n+1/2}, \quad (50)$$

where \mathbf{e}_{B_x} are unit vectors for the magnetic field components in x -direction.

[‡] Note here that we use a consistent superscript (e.g., $\tilde{\mathbf{F}}^*$ and \tilde{E}^*) between the Godunov fluxes and the electric fields that are in the duality relationship. The superscript is used for the intermediate Riemann solutions in Section 2.4, whereas the superscript $*$ (e.g., \mathbf{F}^* and E^*) is used for the final Riemann solutions in Section 2.5.

Now that the second-order accurate Riemann states $\mathbf{V}_{i,j,k,N,S,E,W,T,B}^{n+1/2}$ are available, the second-order Godunov fluxes can be evaluated by solving the last set of Riemann problems at x -interfaces,

$$\mathbf{F}_{i-1/2,j,k}^{*,n+1/2} = \text{RP} \left(\mathbf{V}_{i-1,j,k,E}^{n+1/2}, \mathbf{V}_{i,j,k,W}^{n+1/2} \right), \quad \mathbf{F}_{i+1/2,j,k}^{*,n+1/2} = \text{RP} \left(\mathbf{V}_{i,j,k,E}^{n+1/2}, \mathbf{V}_{i+1,j,k,W}^{n+1/2} \right), \quad (51)$$

Note that the superscript $*$ is used to represent the second-order Godunov fluxes that are the solutions of the Riemann problems.

2.5. Cell-centered Solution Update from n to $n+1$ Time Step

The USM algorithm updates the cell-centered conservative variables to the next time step $n+1$ using an unsplit integrator,

$$\mathbf{U}_{i,j,k}^{n+1} = \mathbf{U}_{i,j,k}^n \frac{\Delta t}{\Delta x} \left\{ \mathbf{F}_{i+1/2,j,k}^{*,n+1/2} - \mathbf{F}_{i-1/2,j,k}^{*,n+1/2} \right\} - \frac{\Delta t}{\Delta y} \left\{ \mathbf{G}_{i,j+1/2,k}^{*,n+1/2} - \mathbf{G}_{i,j-1/2,k}^{*,n+1/2} \right\} - \frac{\Delta t}{\Delta z} \left\{ \mathbf{H}_{i,j,k+1/2}^{*,n+1/2} - \mathbf{H}_{i,j,k-1/2}^{*,n+1/2} \right\}. \quad (52)$$

In general, after this update, non-zero divergence magnetic fields are still present at cell centers, and they need to be corrected. In the next section we update the divergence-free cell face-centered magnetic fields from n to $n+1$ time step using the modified electric field construction (MEC) scheme [40]. The cell face-centered fields are averaged to correct the cell-centered magnetic fields at the $n+1$ state. The choice of a time step Δt for the full 3D CTU scheme is limited by the full CFL bound, with which we set our CFL number to be 0.95 for all numerical results presented in this paper, unless otherwise stated.

2.6. Face-centered, Divergence-Free Fields Update via CT from n to $n+1$ Time Step using MEC

2.6.1. The Standard Arithmetic Averaging Approach in MEC: standard-MEC

In [40], the 2D version of the modified electric field construction (MEC) scheme was introduced. The method provides electric fields at cell corners using high-order Taylor expansions. Displaying the electric field in z -direction only, this standard-MEC algorithm gives

$$\begin{cases} E_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i+1/2,j,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y^2} + O(\Delta y^3), \\ E_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i+1/2,j+1,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y^2} + O(\Delta y^3), \\ E_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x^2} + O(\Delta x^3), \\ E_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i+1,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x^2} + O(\Delta x^3). \end{cases} \quad (53)$$

The duality relationship [5] has been assumed for those electric fields at cell face centers about which the Taylor series are expanded. The standard-MEC algorithm proceeds to take a simple arithmetic average of these four Taylor expansions of each field in Equation (53) to get an averaged electric field $\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2}$.

2.6.2. Upwind Biased Averaging in MEC: upwind-MEC

The standard CT approach of taking the arithmetic average of the four electric fields is simple enough to work well in local smooth regions. The simplest form of this averaging approach was first suggested by Balsara and Spicer [5] using 1D based Riemann solvers. This idea seems a very natural choice if one considers the grid locations of the electric fields. However, the authors understood that in truly multidimensional flows where there is a directional bias, the simple arithmetic averaging scheme may need to be corrected and it would be better to incorporate upwind information. Recently, a general resolution on such issue with multidimensional upwinding has become available by the subsequent efforts to build the genuinely multidimensional HLL-type Riemann solvers by Balsara [10, 11].

On the other hand, within the 1D Riemann based CTU approach, Gardiner and Stone [30] identified the shortcomings of the simple arithmetic averaging method and developed a systematic construction of CT algorithms that are consistent for a plane-parallel, grid-aligned flow. They recovered the necessary amount of numerical viscosity that stabilizes their underlying CT integration algorithm. The CT methods proposed therein readily satisfy planar symmetry for $\partial/\partial x = 0$ or $\partial/\partial y = 0$, showing that their algorithms recover the associated one-dimensional solution for the underlying integration algorithm. A similar approach of increasing dissipation is also found in [45].

Although the approach by Gardiner and Stone provides consistency for plane-parallel, grid-aligned flows, the method does not take into account multidimensional effects where the flow has one specific directional bias without assuming $\partial/\partial x = 0$ or $\partial/\partial y = 0$. To illustrate this, we consider the weakly magnetized field loop advection problem [30, 40] where the loop is advected by a dominant velocity in x and comparably small velocity in y , saying $u > 0$ with $v = \varepsilon > 0$. The simple arithmetic averaging CT algorithm gives

$$\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = \frac{1}{4}(E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i+1/2,j+1,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} + E_{z,i+1,j+1/2,k}^{*,n+1/2}). \quad (54)$$

In the limiting case of $u > 0$ with $v = \varepsilon \rightarrow 0$, it is obvious that $E_{z,i,j+1/2,k}^{*,n+1/2}$ is the only electric field that is in the upwind direction, whereas the rest are not. One can easily see that the similar situation also occurs in the CT scheme in [30]. This suggests that the simple averaging, based on the 1D Riemann solver strategies used with CTU, is potentially exposed to numerical oscillations and therefore its stability is questionable. There are several other modern time-evolution strategies for MHD that do not suffer from this lack of upwinding. As noted, the modern MHD schemes by Balsara [10, 11] using the genuinely multidimensional Riemann solvers evolve the magnetic field structures in any direction without resorting to any added dissipation in the electric fields. The use of multidimensional Riemann solvers for MHD have shown to possess superior capability in evolving magnetic fields to the use of conventional 1D Riemann solvers, better reflecting the true nature of the PDE that does not require any secondary dissipation mechanisms for the purpose of stable upwinding. Although the essential role of the multidimensional technology is acknowledged, our primary goal in this paper is to design an easy alternative that can be ameliorated within the 1D Riemann solver framework based on CTU.

We now describe our new upwind CT construction scheme that resolves this lack of upwind information in the current strategy. As suggested, the idea is to construct the electric fields at $(i + \frac{1}{2}, j + \frac{1}{2}, k)$ including the electric fields at cell interfaces that are in the upwind directions. For example, in the limiting case of $u > 0$ with $v = 0$ the cell-cornered electric field is given by

$$\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i,j+1/2,k}^{*,n+1/2}. \quad (55)$$

Based on this simple idea of upwinding, we illustrate a systematic approach to constructing a new upwind-MEC algorithm that also leads to a consistent CT scheme for plane-parallel, grid-aligned flows. To make our discussion more concise, we display a 2D case; the extension in 3D is straightforward. The first step is to check the upwind direction at each cell corner. This can be done by defining four switches

$$u_P = \frac{1}{2}(1 + \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|, \quad (56)$$

$$u_N = \frac{1}{2}(1 - \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|, \quad (57)$$

$$v_P = \frac{1}{2}(1 + \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|, \quad (58)$$

$$v_N = \frac{1}{2}(1 - \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|, \quad (59)$$

where the sign function is defined by

$$\text{sign}(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x = 0, \\ -1 & \text{if } x < 0. \end{cases} \quad (60)$$

The cell-centered n time step velocity fields are spatially averaged to get the velocities at the cell corner $(i + \frac{1}{2}, j + \frac{1}{2})$ in (56)–(59). When deciding the proper upwind direction at $(i + \frac{1}{2}, j + \frac{1}{2})$ in Equations (56)–(59), it is useful to measure relative magnitudes of velocity fields in order to avoid any numerical noise effects. The small noise perturbations in the signs of velocity fields may lead to an unnecessary amount of changes in upwind directions that are not very advantageous [54]. This motivates to set the velocities at $(i + \frac{1}{2}, j + \frac{1}{2})$ in (56)–(59) to be zero whenever a given local velocity in one direction is relatively small compared to the total local velocity magnitude. That is to say,

$$u_{i+1/2,j+1/2} = 0 \quad \text{if} \quad \frac{|u_{i+1/2,j+1/2}|}{\max(\sqrt{u_{i+1/2,j+1/2}^2 + v_{i+1/2,j+1/2}^2}, \epsilon_2)} \leq \epsilon_1. \quad (61)$$

Notice that the total velocity only includes the two velocity field components u and v (but *not* w) that define the electric field E_z under consideration. Our choice of an empirically derived value ϵ_1 forces to ignore any velocity fluctuations that are smaller than 10% of the total magnitude of velocity fields, and set those velocities to be zero for determining the proper upwind direction. An arbitrary small value is chosen for ϵ_2 to prevent division by zero.

Finally we take an upwind biased averaging of the electric fields using the switches in (56)–(59),

$$\begin{aligned} \tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = & \alpha \left[v_P \left(E_{z,i+1/2,j,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j,k}^{*,n+1/2}}{\partial y^2} \right) + \right. \\ & v_N \left(E_{z,i+1/2,j+1,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1,k}^{*,n+1/2}}{\partial y^2} \right) + \\ & u_P \left(E_{z,i,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) + \\ & \left. u_N \left(E_{z,i+1,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) \right]. \quad (62) \end{aligned}$$

Here the averaging weight factor α is set to 1 if $u_{i+1/2,j+1/2}v_{i+1/2,j+1/2} = 0$; $\alpha = \frac{1}{2}$ otherwise. This is our upwind-MEC scheme. It is interesting to observe that the upwind-MEC scheme satisfies the consistency relationship that reverts to the underlying integration CT scheme for plane-parallel, grid-aligned flows in an upwind sense. To see this we consider for example $\partial/\partial y = 0$. Consider first when $v_{i+1/2,j+1/2} = 0$. In this case the electric fields at each cell corner will take only either the third (if $u_{i+1/2,j+1/2} > 0$) or the fourth (if $u_{i+1/2,j+1/2} < 0$) part of Equation (62). By planar symmetry, $E_{z,i,j+1/2,k}^{n+1/2} = E_{z,i,j,k}^{n+1/2} = E_{z,i,j+1,k}^{n+1/2}$, the first leading terms in both relationships in (62) become

$$\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = \begin{cases} E_{z,i,j+1/2,k}^{*,n+1/2} = E_{z,i,j,k}^{*,n+1/2} & \text{if } u_{i+1/2,j+1/2} > 0, \\ E_{z,i+1,j+1/2,k}^{*,n+1/2} = E_{z,i+1,j,k}^{*,n+1/2} & \text{if } u_{i+1/2,j+1/2} < 0. \end{cases} \quad (63)$$

Therefore they can be considered as an upwind-biased CT variant of $\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i+1/2,j,k}^{*,n+1/2}$ which is the result of the CT method by Gardiner and Stone [30] in this case. If $u_{i+1/2,j+1/2} = 0$ then $\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = 0$

which is an exact solution for ideal MHD[§].

For nonzero values of $v_{i+1/2,j+1/2}$, consider for instance a case for $v_{i+1/2,j+1/2} > 0$ with $u_{i+1/2,j+1/2} > 0$. Then the electric fields from the upwind-MEC scheme will take the parts that have u_P and v_P only, and $\alpha = \frac{1}{2}$. Consider only the first leading terms in the two parts of Equation (62) for an exposition purpose, we get

$$\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = \frac{1}{2} \left(E_{z,i+1/2,j,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} \right) = \frac{1}{2} \left(E_{z,i+1/2,j+1/2,k}^{*,n+1/2} + E_{z,i,j+1/2,k}^{*,n+1/2} \right), \quad (64)$$

where we assumed $\partial/\partial y = 0$ in the last equality. Compared to the electric field $\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} = E_{z,i+1/2,j,k}^{*,n+1/2}$ from the Gardiner and Stone's method, the upwind biased MEC electric field in Equation (64) makes use of an additional upwind electric field at $(i, j + \frac{1}{2}, k)$ and includes that field in the average to get the field at $(i + \frac{1}{2}, j + \frac{1}{2}, k)$.

There are several important features of the upwind-MEC method. First, the method appropriately uses an upwinding direction rather than taking a simple arithmetic average which lacks proper upwinding. The lack of upwinding is found in most of the well known CT schemes [5, 30, 31, 40, 47]. The upwinding strategy becomes most crucial when advecting a magnetized object in one biased direction, for instance, the weakly magnetized field loop advection problem [30] in x -direction only or with a very small advection angle θ relative to x -axis. In this small angle advection case the standard CT update without any upwinding becomes very vulnerable to numerical instabilities that appear as spurious oscillations in the magnetic field evolution. Such oscillations are more likely in the small angle case than in a relatively large angle case because there is only one dominating direction from which the CT electric averaging scheme should rely on to obtain enough numerical dissipation to stabilize the field evolution. It will be shown later that the upwind-MEC strategy advects the field loop without significant numerical oscillations and without distortions for small angle advections.

Second, the upwind-MEC scheme not only accounts for an upwinding direction for stability, but also includes high-order terms. The first derivative terms reflect correct spatial changes in expanding from the center nodes to the corners, while the second terms effectively avoid spurious oscillations near discontinuities by adding the proper amount of numerical dissipation to the corner extrapolated fields [40]. These high-order terms are upwind averaged in such a way that the scheme is consistent for plane-parallel, grid-aligned flows.

Third, as mentioned, the idea of using upwinding in taking the average is to recover a *proper* amount of numerical dissipation required to ensure stability. We note that the greatest benefit occurs when there is a dominating direction locally towards which the magnetic fields are advected. For this reason the upwind-MEC scheme can be turned off when the local flow velocities are all ignorable. When the local velocities are all negligibly small but finite the local flow should be smooth enough, and hence it is sufficiently accurate to use the standard-MEC scheme that takes the arithmetic averaging as discussed in Section 2.6.1. In practice, we switch back to the standard-MEC when the local flow velocities are relatively small compared to the local sound speed C_s . That is, we consider a local Mach number M_z for the local flow switch to choose the standard-MEC for constructing the electric field $\tilde{E}_{z,i+1/2,j+1/2,k}$ if

$$M_z = \frac{\sqrt{u_{i+1/2,j+1/2}^2 + v_{i+1/2,j+1/2}^2}}{C_s} \leq \epsilon_3. \quad (65)$$

[§] Note that for non-ideal MHD the upwinding approach in the upwind-MEC scheme should only be applied to the induction part (i.e., $-\mathbf{u} \times \mathbf{B}$) of a generalized Ohm's law including the terms such as the magnetic diffusion, the Hall effect and the Biermann battery effect.

An empirical based tunable parameter $\epsilon_3 = 10^{-4}$ suffices to detect a local smooth flow in order to convert back to the standard-MEC method; otherwise the upwind-MEC scheme is enabled for all the numerical tests presented in this paper.

2.6.3. CT Update from n to $n+1$ Time Step

Using the electric fields $\tilde{E}_{x,i,j+1/2,k+1/2}^{n+1/2}$, $\tilde{E}_{y,i+1/2,j,k+1/2}^{n+1/2}$ and $\tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2}$ constructed by our MEC strategy, the final CT update evolves the cell face-centered magnetic fields satisfying the $\nabla \cdot \mathbf{B} = 0$ condition on a staggered grid. Displaying only in x -direction, we have

$$b_{x,i+1/2,j,k}^{n+1} = b_{x,i+1/2,j,k}^n - \frac{\Delta t}{\Delta y} \left\{ \tilde{E}_{z,i+1/2,j+1/2,k}^{n+1/2} - \tilde{E}_{z,i+1/2,j-1/2,k}^{n+1/2} \right\} - \frac{\Delta t}{\Delta z} \left\{ -\tilde{E}_{y,i+1/2,j,k+1/2}^{n+1/2} + \tilde{E}_{y,i+1/2,j,k-1/2}^{n+1/2} \right\}. \quad (66)$$

This completes our description of all procedures in the 3D USM algorithm for a single time step update.

3. Summary

We summarize the 3D USM algorithm as follows:

- (i) Calculate the normal predictor states in all x, y, z -directions using the algorithm described in Section 2.2. When calculating the normal state in each direction, include the associated MHD term that is proportional to the gradient of the normal field, see the first relation in (19). During each normal predictor calculation, the eigensystems in the normal direction are to be computed. They are stored for later use in the transverse correctors. At the same time, the summations of the jumps in all characteristic variables are also computed and stored, see Equations (26)-(27), the pseudo-code in Section 2.3.1, the sigma summations in Equations (45) and (47).
- (ii) The normal predictor states are updated via the transverse correctors described in Section 2.3.2. This step uses two of the stored sigma summation terms that are calculated and stored in each normal predictor step. The summations reflect the transverse flux gradients using the characteristic tracing approach.
 - (a) The reduced 3D CTU scheme then proceeds to advance the normal fields by half a time step using CT as illustrated in Section 2.4, finalizing all the interface state calculations. In the reduced 3D CTU scheme, the formal stability limit is given by a CFL number that is less than $\frac{1}{2}$.
 - (b) If the full 3D CTU scheme is chosen, the algorithm needs to take one more correction step, presented in Section 2.3.3. This correction step is essential in order to provide the full stability limit by including the diagonally moving upwind information along the corners in a 3D control volume. Similar to the reduced CTU scheme, the full 3D CTU scheme is completed by evolving the cell face-centered magnetic fields by half a time step as in Section 2.4.

So far, both of the two CTU algorithms have required the first set of three Riemann problems that are used to advance the magnetic fields by CT.

- (iii) Solve the final set of three Riemann problems at cell interfaces and update the cell-centered conservative variables to the next time step as described in Section 2.5. The total number of Riemann solves therefore becomes six[¶].
- (iv) Calculate the electric fields at cell corners by using the upwind-MEC algorithm described in Section 2.6.2. With these electric fields, the magnetic fields at cell face centers are updated to the next time

[¶] Our unsplit data reconstruction-evolution algorithm can be easily modified for use as a gas hydrodynamics solver by omitting those steps related to the magnetic fields. In this case, there are only three Riemann solves required as there is no CT update needed. This unsplit hydrodynamics solver has been also available in FLASH's official releases.

step by CT. The cell-centered magnetic fields are updated by taking arithmetic averages of these divergence-free magnetic fields at cell face centers (e.g., Equation (21) in Section 2.2).

4. Numerical Results

In this section we exhibit the accuracy, stability, convergence and computational performance of the USM scheme on a suite of 3D MHD problems. These results show that the scheme is very robust with the full CFL stability bound. The scheme is second-order accurate for smooth flows and maintains the solenoidal constraint on the magnetic field up to machine round-off error. The full 3D CTU method is our primary default method for which a CFL number of 0.95 is chosen in all of the simulations presented here. We also show a set of comparison studies between the reduced and full 3D CTU schemes. Insofar as choice of Riemann solver is concerned, we use the Roe-type linearized solver [53,63] and the HLLD solver [48]. Our choices for the normal predictor step are MUSCL-Hancock, PPM, and WENO5.

4.1. Field Loop Advection

This problem is notoriously difficult to solve, not because of any strong shock causing numerical instability and leading to code to crash, but rather because it requires full accounting of multidimensional advection in a stable matter, such as including the multidimensional MHD terms [30, 31, 40, 47]. Failure to do so results in an erroneous generation of in-plane magnetic field, which results in the distortion of the initially circular (2D) or cylindrical (3D) field loop.

In addition to the standard field loop advection case studied in [31], we also consider a small angle advection case. This turns out to be a much more stringent test than the standard advection configuration which assumes a (relatively) large angle between the advection flow and the Euclidean coordinate axes. In the small angle configuration there is one dominating coordinate direction along which the field loop is advected. This means that, in practice, there is only one direction from which a numerical scheme can obtain the numerical dissipation required for stability. In multidimensional problems, inadequate numerical dissipation from transverse directions can give rise to anomalous oscillatory behavior in physical variables.

We begin by describing the initial setup for the standard large angle advection case following the configuration of [31]. The weakly magnetized 3D cylindrical field loop is initialized with a very high plasma beta $\beta = p/B_p = 2 \times 10^6$ in the inner region, where $B_p = (B_1^2 + B_2^2 + B_3^2)/2$. Inside the loop the magnetic field strength is very weak and the flow dynamics are dominated by the gas pressure.

The initial field loop is tilted around the x_2 (or y) axis by $\omega = \tan^{-1} \Omega$ radians in a 3D periodic box $[-0.5, 0.5] \times [-0.5, 0.5] \times [-1, 1]$. For the standard large angle setup, we choose $\Omega = 2$. The field loop is frozen into the ambient plasma and is advected diagonally across the domain with the plasma advection velocity $(u, v, w) = (1, 1, 2)$. The density and pressure are equal to unity everywhere, and $\gamma = \frac{5}{3}$.

The magnetic field components are initialized by taking numerical curl of the magnetic vector potential $\mathbf{A} = (A_1, A_2, A_3)^T$ in order to ensure $\nabla \cdot \mathbf{B} = 0$ initially. The relationship between magnetic field and vector potential gives

$$B_1 = \frac{\partial A_3}{\partial x_2} - \frac{\partial A_2}{\partial x_3}, \quad B_2 = -\frac{\partial A_3}{\partial x_1} + \frac{\partial A_1}{\partial x_3}, \quad B_3 = \frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2}. \quad (67)$$

For the components of \mathbf{A} we choose $A_1 = A_2 = 0$ and

$$A_3 = \begin{cases} A_0(R - r) & \text{if } r \leq R, \\ 0 & \text{otherwise.} \end{cases} \quad (68)$$

By using this initialization process divergence-free magnetic fields are well constructed numerically on a staggered grid. The parameters in Equation (68) are $A_0 = 10^{-3}$ and $R = 0.3$.

The two coordinate systems (x_1, x_2, x_3) and (x, y, z) are related by a rotation about the y -axis, which is given by

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \cos\omega & 0 & \sin\omega \\ 0 & 1 & 0 \\ -\sin\omega & 0 & \cos\omega \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \quad (69)$$

Before we present the standard large angle field loop advection, we first consider a small angle advection case in 2D. The 2D initial conditions can be found in [30, 40] and we will not repeat the details here. In the 2D setup, the velocity field is given by

$$\mathbf{U} = (u_0 \cos\theta, u_0 \sin\theta, 1)^T, \quad (70)$$

where $u_0 = \sqrt{5}$. We chose $\theta = \tan^{-1}(0.01) \approx 0.573^\circ$ for a small angle advection test. With this setup, the field loop is advected almost entirely in the positive x -direction. This situation makes it hard to stabilize the solution during advection because there is not enough numerical dissipation from the y -direction. The solution behavior completely relies on the dissipation mechanism from the x -direction only, making the problem very unstable if no special care is taken to stabilize it.

In Figure 2, we illustrate the evolution of the magnetic pressure B_p at $t = 0.1$ and 2.0 using the upwind-MEC scheme described in Section 2.6.2. In consequence of the upwinding dissipation mechanism, the upwind-MEC scheme stabilizes the solutions extremely well, suppressing the anomalous behavior during the advection.

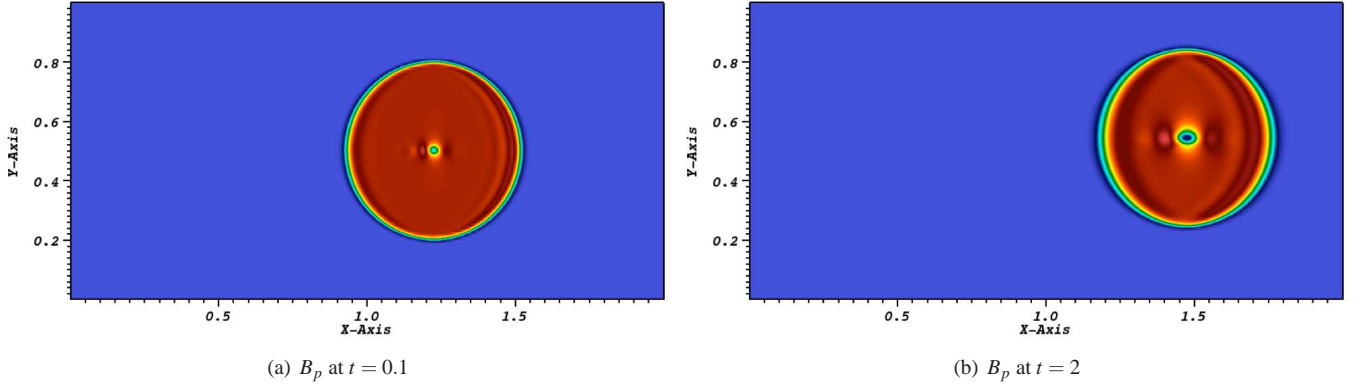


Fig. 2. The 2D field loop advection using a small advection angle $\theta \approx 0.573^\circ$ relative to the x -axis. The images are magnetic pressures at times $t = 0.1$ and 2 using PPM and the Roe Riemann solver. The minmod slope limiter is used for taking slope gradients of characteristic variable in the PPM reconstruction step. All results are resolved on 200×100 grid cells using the upwind-MEC scheme.

In Figure 3 (a), the small angle advection test is repeated in 3D, whereas a large angle advection is demonstrated in Figure 3 (b). The velocity fields are respectively given by $\mathbf{U} = (\cos\theta, \sin\theta, 2)^T$ and $\mathbf{U} = (1, 1, 2)^T$ for the small and large angle runs. In (a), the same small advection angle $\theta \approx 0.573^\circ$ was used relative to the x -axis as in the 2D case. In the large angle case in (b), the field loop makes a domain diagonal advection from the given initial velocity condition. We set the tilt angle ω in Equation (69) to be same as θ for both (a) and (b). In both runs, we show that the upwind-MEC scheme manifests an oscillation-free advecting, well-preserving the initial cylindrical shape in the magnetic pressure as shown. As noted above, numerical dissipation in the large angle run is naturally added from all directions, rather than from one specific direction along the advection in the small angle case. Such added dissipation makes the large angle case easier to demonstrate than the small angle case.

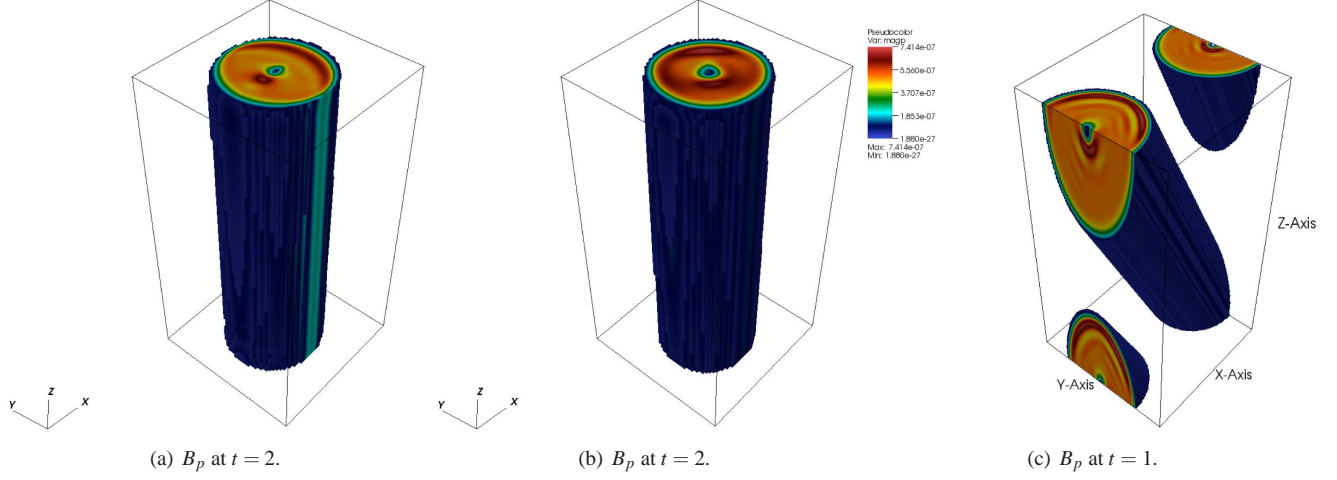


Fig. 3. (a) 3D field loop advection using a small advection angle $\theta \approx 0.573^\circ$ relative to the x -axis. (b) 3D field loop advection using a large advection angle using $\mathbf{U} = (1, 1, 2)^T$. (c) The standard field loop advection problem at time $t = 1$. All results use PPM and the Roe Riemann solver, and the minmod slope limiter on characteristic variables in the PPM reconstruction. The results in (a) and (b) are resolved on $64 \times 64 \times 128$ grid cells, and (c) on $128 \times 128 \times 256$. The upwind-MEC is used in all cases.

As a final test in this section, we perform the standard field loop advection problem in Figure 3 (c), following the configuration in [31]. We see that the upwind-MEC scheme performs very well in evolving the field loop successfully to the final time $t = 1$. This result in (c) can be directly compared to the results reported in [31]. We also report that the upwind-MEC scheme increases the maximum value of the magnetic pressure by 48% to 7.41×10^{-7} from its initial value of 5×10^{-7} . The larger growth of the maximum value is found in the standard-MEC scheme, increasing the initial value by 69% (not shown here).

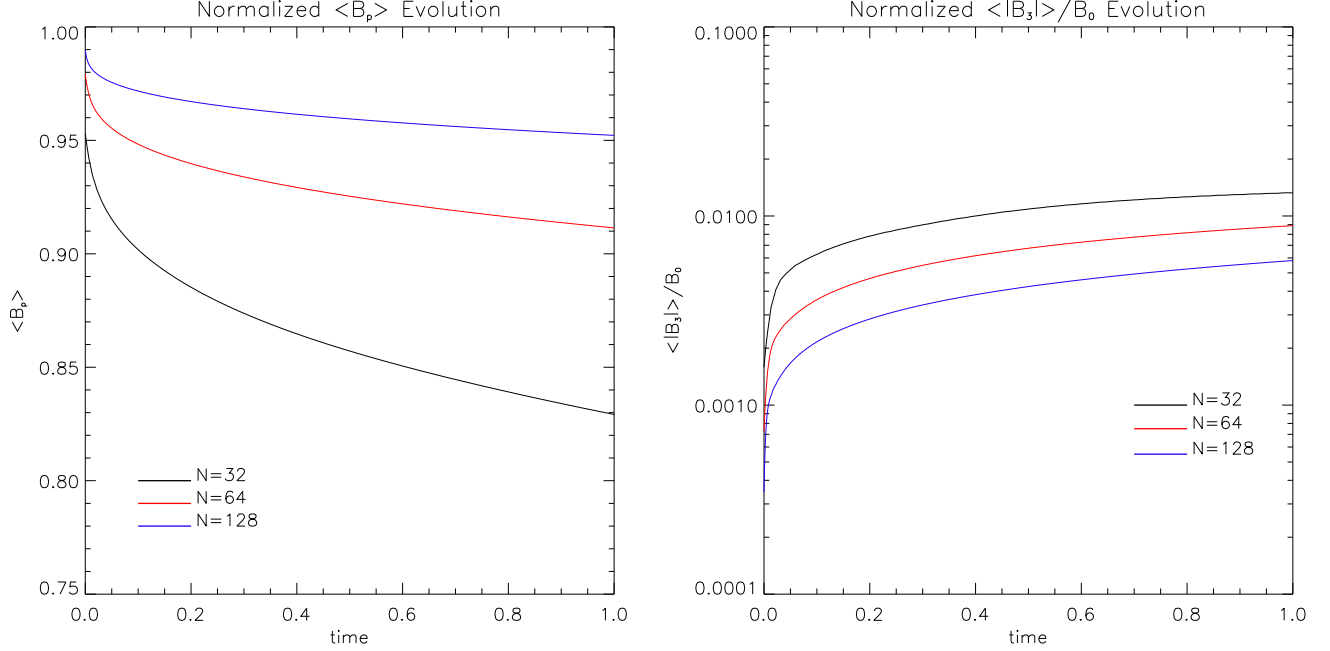
Furthermore, we present two quantitative results in Figure 4. They include (a) the temporal evolution of the volume-averaged magnetic energy density normalized to the initial (analytic) value $\langle B_p \rangle = \langle B^2 \rangle = B_0^2 \sqrt{5} \pi R^2 / 2$; and (b) the temporal evolution of the normalized error $\langle |B_3| \rangle / B_0$. Both results in (a) and (b) are similar to those reported in [31, 47]. However in (b), the final values at $t = 1$ are found out to be little larger than those in [31, 47] at each grid resolution. This is probably because our full 3D CTU method of including the MHD multidimensional terms ignores the $O(\Delta t)$ terms in evaluating the eigensystems of the \mathbf{A}_d matrices at $n + \frac{1}{3}$ (see for example Equation (35)), where $d = x, y, z$.

4.2. Circularly Polarized Alfvén Wave

In the next test we solve the circularly polarized Alfvén wave and its propagation [30, 31, 65]. This problem provides an important quantitative test of the 3D USM scheme because the smooth initial conditions are nonlinear solutions to the problem. The Alfvén wave propagates parallel to the x_1 -axis of a transformed coordinate system (x_1, x_2, x_3) in the periodic computational domain $[0, 3] \times [0, 1.5] \times [0, 1.5]$. The computational domain is resolved on $2N \times N \times N$ grid cells, where we adopt $N = 8, 16, 32$ and 64 for the convergence study.

The relationship between the rotated coordinated system (x, y, z) and the non-rotated system (x_1, x_2, x_3) is described by the following coordinate transformation

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x \cos \alpha \cos \beta + y \cos \alpha \sin \beta + z \sin \alpha \\ -x \sin \beta + y \cos \beta \\ -x \sin \alpha \cos \beta - y \sin \alpha \sin \beta + z \cos \alpha \end{pmatrix}, \quad (71)$$



(a) Normalized, volume averaged magnetic energy density in time

(b) Normalized B_3 error in time

Fig. 4. Time evolution of (a) the normalized, volume averaged magnetic energy density $\langle B_p \rangle = \langle B^2 \rangle$ and (b) the normalized error $\langle |B_3| \rangle / B_0$. Three different results on the grid resolutions of $N = 32, 64$ and 128 are plotted. The full CTU scheme is adopted with $CFL=0.95$ using PPM and the Roe Riemann solver.

where $\sin \alpha = \frac{2}{3}$, $\sin \beta = \frac{2}{\sqrt{5}}$, $\cos \alpha = \frac{\sqrt{5}}{3}$, and $\cos \beta = \frac{1}{\sqrt{5}}$.

The initial conditions we use are the same as the equivalent test problems described in [31]. The initial magnetic field is given by

$$\mathbf{B} = (B_{x_1}, B_{x_2}, B_{x_3})^T = (1, 0.1 \sin(2\pi x_1/\lambda), 0.1 \cos(2\pi x_1/\lambda))^T, \quad (72)$$

and similarly the velocity field is

$$\mathbf{U} = (U_{x_1}, U_{x_2}, U_{x_3})^T = \begin{cases} (0, 0.1 \sin(2\pi x_1/\lambda), 0.1 \cos(2\pi x_1/\lambda))^T & \text{for traveling wave,} \\ (1, 0.1 \sin(2\pi x_1/\lambda), 0.1 \cos(2\pi x_1/\lambda))^T & \text{for standing wave.} \end{cases} \quad (73)$$

We set the wavelength $\lambda = 1$. The density and the gas pressure are initialized by $\rho = 1$ and $p = 0.1$. We choose PPM and the HLLD Riemann solver, with the monotonized central (MC) limiter.

Figure 5 (a) and (b) show the numerical errors on a logarithmic scale obtained with four different grid resolutions of $N = 8, 16, 32$ and 64 . We test the reduced 3D CTU scheme using $CFL=0.475$ and the full 3D CTU scheme using $CFL=0.475$ and 0.95 for the convergence study. The errors of the standing and traveling waves are plotted in (a) and (b) respectively. For all cases we follow the error calculation formula used by Gardiner and Stone [31] in order to compare our results with theirs. The results in Figure 5 (a) and (b) show a second-order convergence rate of both reduced and full 3D CTU schemes for the smooth Alfvén wave problem.

We also measure the relative CPU cost of the full CTU scheme to the reduced CTU scheme, $CPU_{rel} = CPU_{f-ctu}/CPU_{r-ctu}$. We find that CPU_{rel} is about 0.8 on average, which indicates that our full CTU scheme with a higher CFL number (e.g., 0.95) is 20% more computationally efficient than the reduced CTU with a lower CFL number (e.g., 0.475). The equivalent performance comparison is different in the 6-solve and the 12-solve algorithms in [31] in that their relative CTU performance turns out to be 1.

As the error magnitudes are nearly identical for both standing and traveling wave modes in the reduced CTU with CFL=0.475 and the full CTU with CFL=0.95, we conclude that our full 3D CTU scheme exhibits better performance while providing numerical solutions that are second-order accurate.

The figures exhibit a dependence of the truncation error in the full CTU scheme on CFL, in both wave modes. The error corresponding to CFL=0.475 is smaller in the standing wave, whereas it is larger in the traveling wave simulation. This type of CFL dependence is also seen in [31].

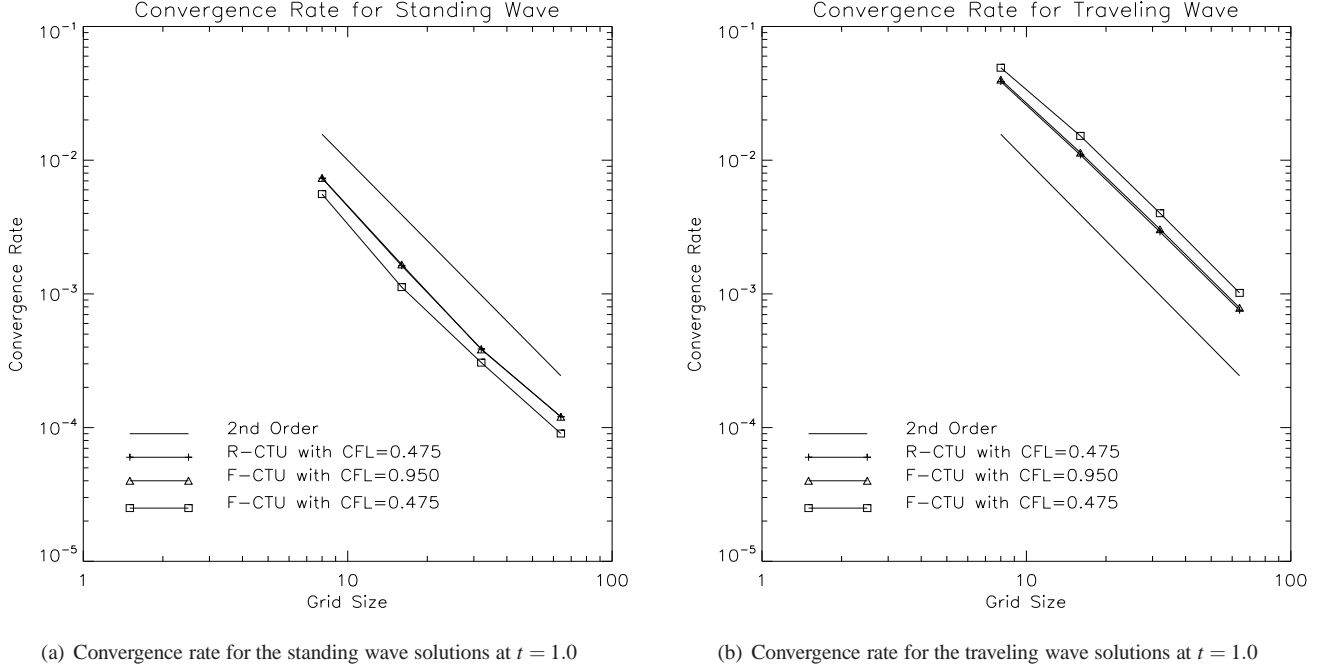


Fig. 5. The circularly polarized Alfvén wave convergence rate for both the standing and traveling wave problems. PPM is used along with the HLLD Riemann solver.

4.3. Orszag-Tang Problem

The third test problem is the Orszag-Tang MHD vortex problem [49]. We follow the 3D extension [36] of the 2D problem in which the initial velocity field is slightly perturbed by ε in the vertical direction. That is, the initial velocity field defined on a periodical computational domain $[0, 1] \times [0, 1] \times [0, 1]$ is written as

$$\mathbf{U} = (-(1 + \varepsilon \sin 2\pi z) \sin 2\pi y, (1 + \varepsilon \sin 2\pi z) \sin 2\pi x, \varepsilon \sin 2\pi z)^T, \quad (74)$$

where we use $\varepsilon = 0.2$ as in [36]. The rest are initialized similar to the 2D case so that

$$\rho = \gamma^2, \quad p = \gamma, \quad \mathbf{B} = (-\sin 2\pi y, \sin 4\pi x, 0)^T, \quad (75)$$

where $\gamma = \frac{5}{3}$. As in the 2D case, the plots in Figure 6 exhibit nonlinear steepening that builds strong discontinuities from the smooth initial conditions. We show the evolutions of density at $t = 0.5$ and 1.0 on 128^3 grid cells. The density images at the top of the domain are very similar to those in the standard 2D case at each corresponding time (e.g., see [40]). The flow symmetries are also well preserved in (b) where density has developed into more complicated discontinuous flows. The Roe Riemann solver is used with the PPM scheme for data reconstruction-evolution in normal direction with MC limiter.

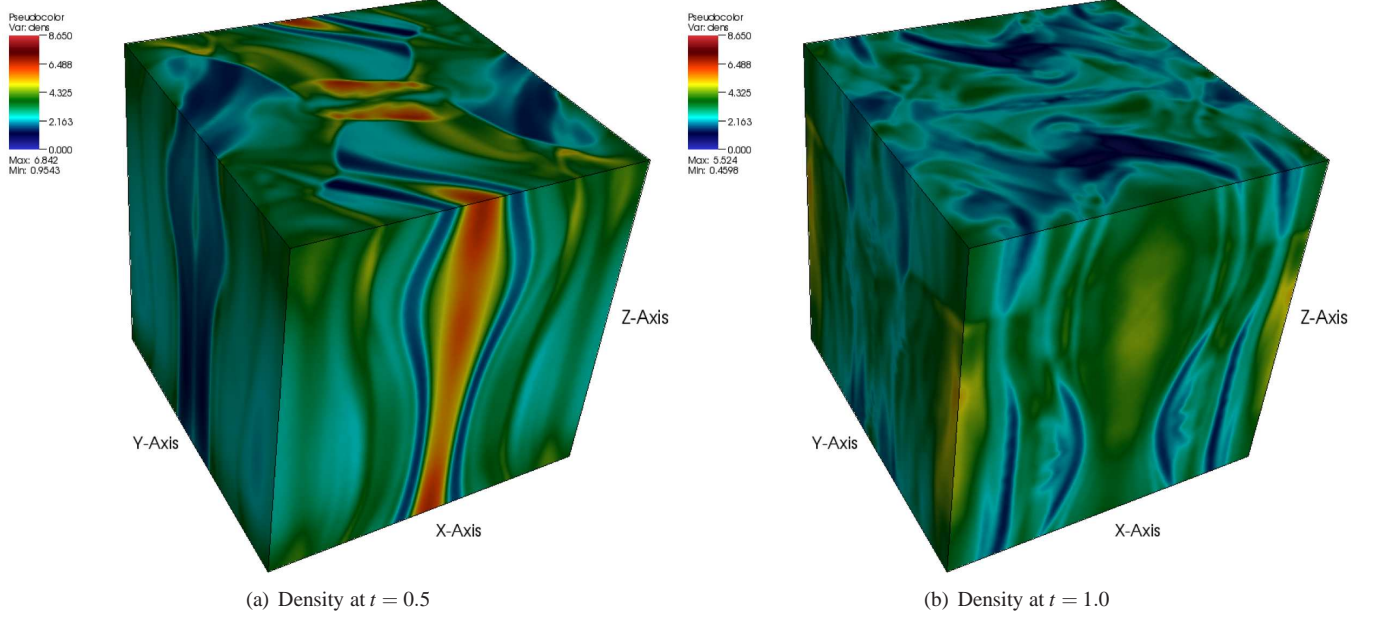


Fig. 6. Density plots of the Orszag-Tang problem at a resolution of 128^3 .

4.4. Rotor Problem

We extend the 2D rotor problem [5, 40, 65] to a 3D case by applying a small velocity perturbation analogous to that introduced in the 3D Orszag-Tang problem in Section 4.3. A dense rotating cylinder is initialized on a unit cube domain $[0, 1] \times [0, 1] \times [0, 1]$ with non-reflecting boundary conditions. The initial velocity field is defined by

$$\mathbf{U} = (u_{2d}(1 + \varepsilon \sin 2\pi z), v_{2d}(1 + \varepsilon \sin 2\pi z), \varepsilon \sin 2\pi z)^T, \quad (76)$$

where $\varepsilon = 0.3$ and

$$u_{2d} = \begin{cases} -f(r)u_0(y - 0.5)/r_0 & \text{for } r \leq r_0 \\ -f(r)u_0(y - 0.5)/r & \text{for } r_0 < r < r_1, \\ 0 & \text{for } r \geq r_1 \end{cases} \quad (77)$$

$$v_{2d} = \begin{cases} f(r)u_0(x - 0.5)/r_0 & \text{for } r \leq r_0 \\ f(r)u_0(x - 0.5)/r & \text{for } r_0 < r < r_1. \\ 0 & \text{for } r \geq r_1 \end{cases} \quad (78)$$

The density, pressure, magnetic field, and the parameters are initialized as in the standard 2D case given by

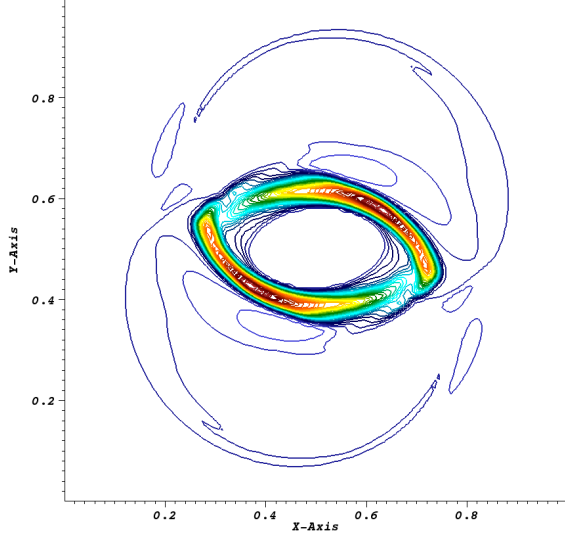
$$\rho = \begin{cases} 10 & \text{for } r \leq r_0 \\ 1 + 9f(r) & \text{for } r_0 < r < r_1, \\ 1 & \text{for } r \geq r_1 \end{cases} \quad (79)$$

$$p = 1, \mathbf{B} = (5/\sqrt{4\pi}, 0, 0)^T, \quad (80)$$

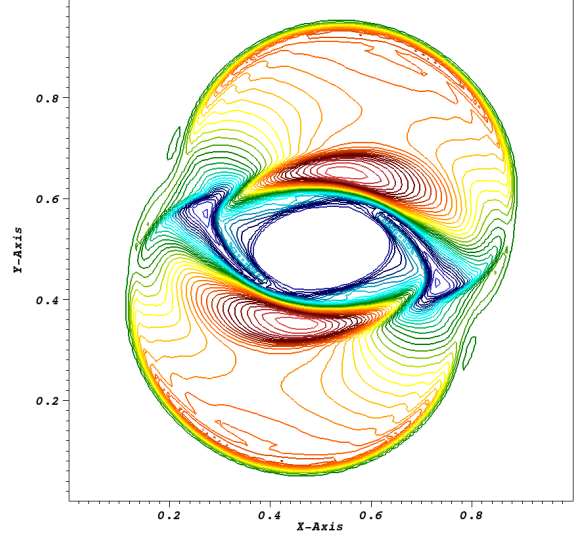
where $u_0 = 2, r_0 = 0.1, r_1 = 0.115, r = \sqrt{(x - 0.5)^2 + (y - 0.5)^2}$, and the taper function $f(r)$ is defined by $f(r) = (r_1 - r)/(r_1 - r_0)$. The value $\gamma = 1.4$ is used.

Panels in Figure 7 exhibit contour plots in x - y plane of the density, magnetic pressure and Mach number at the final time $t = 0.15$. Contour slices are taken at $z = 0.5$. The problem is solved on a 128^3 grid resolution

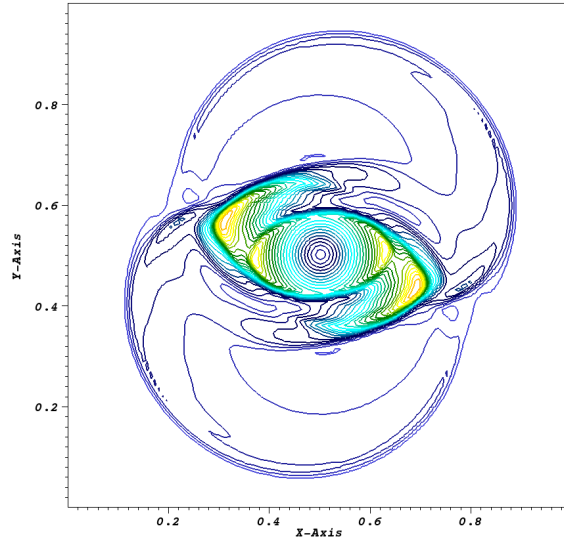
using the Roe solver with PPM. MC limiter is used for the PPM reconstruction. For all cases 40 equally spaced contour lines are plotted. All of the contour plots show that our 3D results correspond very closely to the underlying 2D solutions (e.g., see [40]). As reported in [65] one important feature to observe in this problem is to check the oval contours of Mach number near the center. As illustrated, the contour lines are symmetrical and well preserved with our choice of CFL=0.95.



(a) Density contour at $z = 0.5$ ranging between 0.4540 and 14.82



(b) Magnetic pressure contour at $z = 0.5$ ranging between 0.009705 and 3.171



(c) Mach number contour at $z = 0.5$ ranging between 3.268×10^{-5} and 5.938

Fig. 7. The rotor problem with a resolution of 128^3 at $t = 0.15$. In all cases, 40 equally spaced contour lines are plotted.

4.5. Cloud & Shock Interaction

In the next test problem we consider the interaction of a high density cloud with a strong shock wave, originally studied by Dai and Woodward [19] and often referred to as the cloud-shock interaction problem. This problem aims to test the code robustness in solving flow conditions such as high supersonic Mach numbers in the pre-shock and the post-shock regions, wide ranges of plasma beta values across the front/rear of the cloud, and strong shear flows [36, 40, 47, 65].

Our computational domain is a cube, spanning from -0.5 to 0.5 in all three directions and is resolved on 128^3 grid cells. Supersonic inflow boundary conditions are imposed at the lower boundary $x = -0.5$, while outflow conditions are used elsewhere. The initial condition has different left and right states, separated by an initial discontinuity at $x = 0.1$, given by

$$(\rho, u, v, w, B_x, B_y, B_z, p) = \begin{cases} (3.86859, 0, 0, 0, 0, 2.1826182, -2.1826182, 167.345) & \text{if } x \leq 0.1, \\ (1, -11.2536, 0, 0, 0, 0.56418958, 0.56418958, 1) & \text{if } x > 0.1. \end{cases} \quad (81)$$

The high density cloud is located on the right side of the domain, and has a spherical envelope defined by $(x - 0.3)^2 + y^2 + z^2 = 0.15^2$. A uniform density $\rho = 10$ and pressure $p = 1$ are fixed in the inner region of the cloud, and $\gamma = 5/3$ is used everywhere. The velocity and the magnetic fields are the same as the surrounding right state plasma values. The simulation is carried out to a final time $t = 0.06$ using the WENO5 reconstruction scheme and the Roe Riemann solver. We used the van Leer's slope limiter for limiting characteristic variables in the WENO5 reconstruction.

Figure 8 shows density (plotted in the top half using a red color scheme) and magnetic pressure (plotted in the bottom half using a blue color scheme) at $t = 0.06$. The main features of the cloud-shock interaction process are well captured, in that the temporal evolution of the high density cloud produces disrupted shapes as the cloud moves into the plane shock on the left.

Simulations of this problem are often performed using a rather diffusive set of numerical options such as the minmod slope limiter, HLL-type Riemann solvers, or lower values of CFL. For example, as noted by Tóth, dimensionally-split MHD algorithm can easily fail due to unphysical states (e.g., negative pressure or density) arising in consequence of the strong interaction between the shock and the cloud. By contrast, the 3D USM scheme utilizing the full 3D CTU algorithm and the upwind-MEC scheme can run this simulation successfully without relying on such numerically dissipative choices. Despite our choice of the van Leer's limiter for WENO5, and of the Roe Riemann solver using CFL=0.95, the final time step is reached successfully without giving rise to any numerical instabilities.

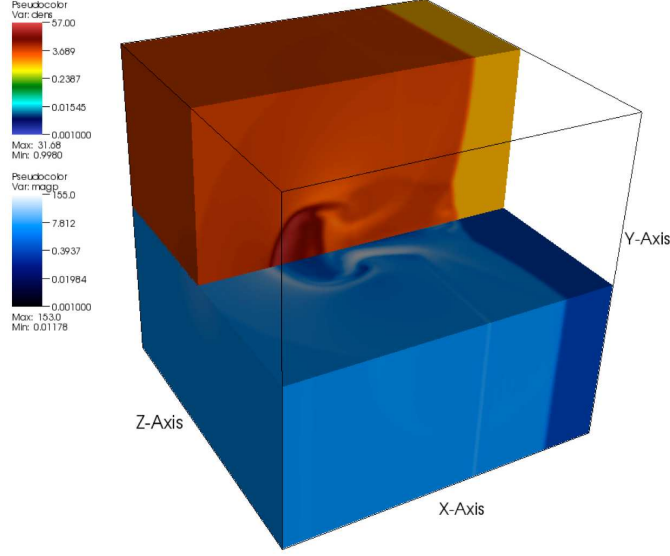
4.6. MHD Blast Wave

The last test case is the 2D MHD spherical blast wave problem of Zachary *et al.* [68]. We presented our 2D results in [40] and extend the problem to 3D here. We test three different configurations, differing by the initial strength of magnetic field in x -direction, each leading to strong shock formation and propagation.

The computational domain is a unit cube $[-0.5, 0.5] \times [-0.5, 0.5] \times [-0.5, 0.5]$ with a grid resolution of 128^3 . The ambient gas is initialized as

$$\rho = 1, p = 0.1, \mathbf{B} = (B_{x_0}, 0, 0)^T, \quad (82)$$

where the three simulations have initial values of B_{x_0} given by $B_{x_0} = 0$, $B_{x_0} = \frac{50}{\sqrt{4\pi}}$ and $B_{x_0} = \frac{100}{\sqrt{4\pi}}$. At the center of the domain, a spherical region of radius $r = 0.1$ is initialized with a very strong pressure $p = 1000$. The non-zero values of $B_{x_0} = \frac{50}{\sqrt{4\pi}}$ and $\frac{100}{\sqrt{4\pi}}$ produce very low- β ambient plasma states, $\beta = 1 \times 10^{-3}$ and 2.513×10^{-4} respectively. Through these low- β ambient states, the explosion initially emits almost spherical fast magneto-sonic shocks that propagate with the fastest wave speed. The flow has $\gamma = 1.4$.



(a) Density and magnetic pressure at $t = 0.06$

Fig. 8. The 3D MHD interaction between the high density cloud and shock structures resolved on 128^3 grid using the Roe Riemann solver and the 5th order WENO scheme. Plotted are density (denoted as "dens" in the legend) in the top half and magnetic pressure (denoted as "magp") in the bottom half.

Shown in Figures 9–11 are (a) density (plotted in the top half) and magnetic pressure (plotted in the bottom half) and (b) contour plots of gas pressure (top half) and total velocity $U = \sqrt{u^2 + v^2 + w^2}$ (bottom half) at time $t = 0.01$. The contour slice plots are the x - y planes taken at $z = 0$.

This problem is susceptible to a type of shock wave instability known as the carbuncle phenomenon [52]. The carbuncle instability takes place in multidimensional numerical solutions when using a less dissipative, 1D based (rather than the multidimensional based [10]) Roe-type Riemann solver, in the regions where a planar shock is aligned to the grid. The cause of this instability is the lack of numerical diffusivity added to the Roe-type fluxes perpendicular to the grid-aligned shock, resulting in a growth of small amplitude noise in the transverse direction. There are several approaches to fix the instability [33, 50, 56, 59] which all basically provide a similar mechanism to add extra numerical diffusion in the transverse direction. Here we use a hybrid Riemann solver that appropriately combines Roe and HLLE depending on the strength of shocks. In this approach, the HLLE solver is adaptively used only in strong shock fronts detected by a shock switch [5]; the Roe solver is used elsewhere. The second-order accurate MUSCL-Hancock scheme is used for the normal predictor calculations. We also employ a hybrid-type of slope limiter that combines MC limiter for linearly degenerate waves (i.e., Alfvén and entropy waves) and the minmod limiter for genuinely nonlinear waves (i.e., magneto-sonic fast and slow waves). This hybrid limiter approach provides an added robustness and accuracy by using a compressive limiter (such as MC and van Leer's) for crisper representation of the linear waves, whereas a diffusive limiter (such as minmod) for the self-steepening nonlinear waves [7].

The case $B_{x_0} = 0$ is illustrated in Figure 9. The carbuncle phenomenon can appear to be stronger in this hydrodynamic limit than when $B_{x_0} \neq 0$. Using the hybrid Riemann solver, however, we do not see any artifacts at the shock fronts that are aligned to the grid axes. In the absence of magnetic field the explosion propagates the shock wave spherically in all radial directions, as exhibited in the contour plots in Figure 9 (b).

In Figure 10 the intermediate magnetic field strength case with $B_x = \frac{50}{\sqrt{4\pi}}$ is shown. The explosion becomes

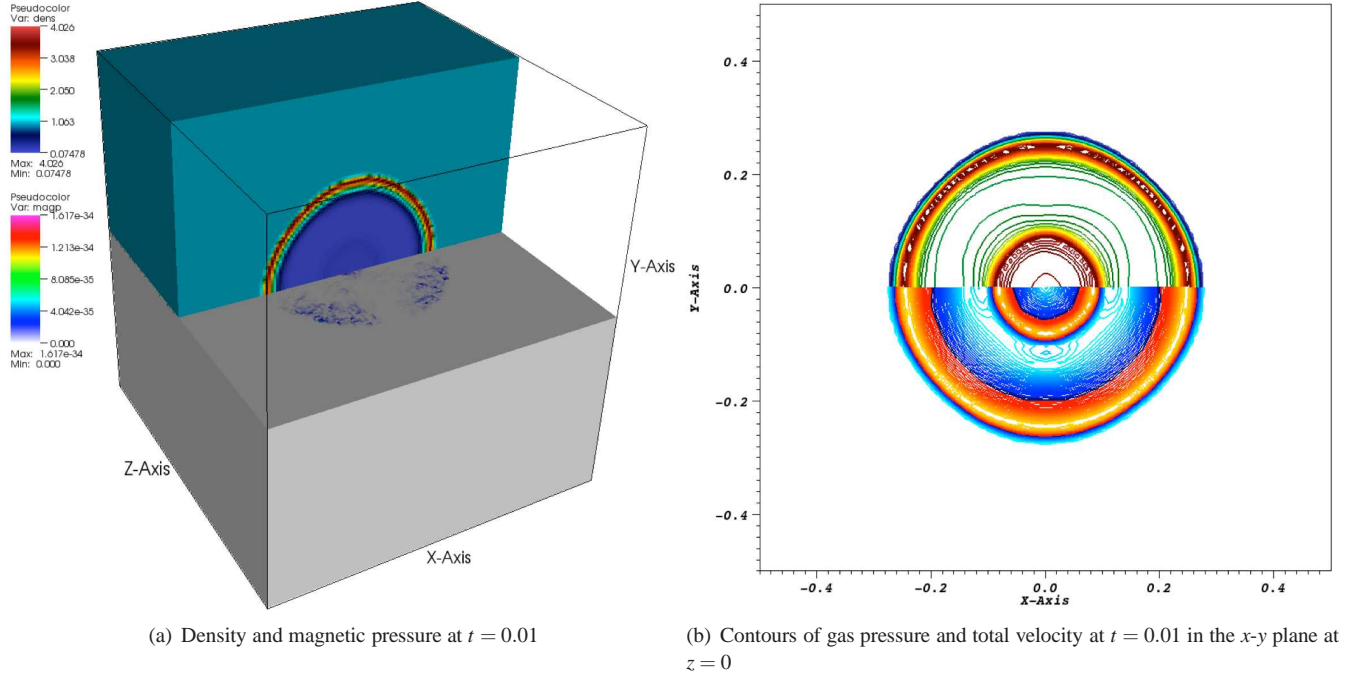


Fig. 9. Results of the blast problem simulation with $B_x = 0$ using a hybrid Riemann solver. In (a), density (denoted as "dens" in the legend) is plotted at the top half. Magnetic pressure (denoted as "magp" in the legend) is plotted at the bottom half and is represented as small values that are numerical noise. In (b), 40 contour lines are plotted for gas pressure (top half) between 0.1 and 73.62 and total velocity (bottom half) between 0 and 8.810.

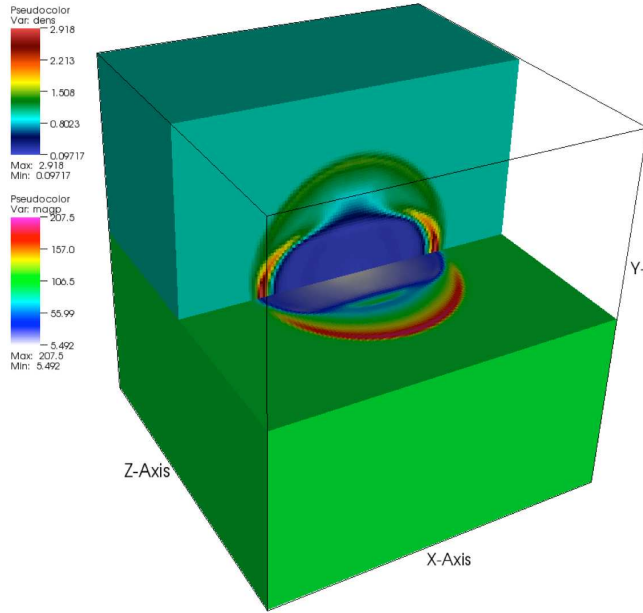
anisotropic because of the non-zero magnetic field strength in x -direction. The intermediate value of B_x still permits shock wave propagation in the y -direction, so that the overall spherical shape is not radically distorted. Nonetheless, the development of the elongated wave structures in the direction parallel to the B_x field is evident compared to the hydrodynamic limit case in Figure 9.

Finally, Figure 11 illustrates the strongest magnetic field case, $B_x = \frac{100}{\sqrt{4\pi}}$. The explosion now becomes highly anisotropic. This strong anisotropic behavior is well shown in Figure 11(b) in that the displacement of gas in the transverse y -direction is increasingly inhibited and hydrodynamical shocks propagate almost entirely in the x -direction parallel to B_x . It is also evident that several weak magneto-sonic waves are radiated transverse to the x -direction. This process continues until total pressure equilibrium is reached in the central region.

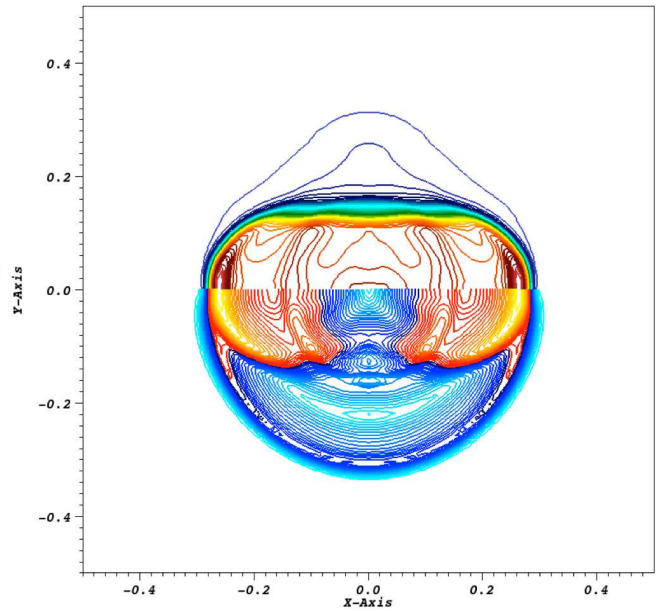
Balsara [7] pointed out that maintaining positivity of pressure becomes challenging due to the strong wave propagation oblique to the mesh. Such unphysical pressures can distort contours, especially near the outer boundary where a large and unphysical drop in pressure takes place immediately ahead of the shock. In our calculations, the pressure remains always positive throughout the simulations, evidence that our 3D MHD scheme is very robust and accurate with our choice of high CFL=0.95.

5. Conclusion

We summarize several key features described in this paper. First, the 3D USM scheme has been introduced, developed and studied. The method is a 3D extension of the 2D USM algorithm [40] which employs characteristic analysis to account for contributions of both normal and transverse MHD fluxes in a truly unsplit fashion. Therefore they do not need intermediate Riemann solves to correct the normal predictor states with the transverse flux updates as in the usual 12-solve CTU algorithm [47, 55]. Our approach of using characteristic analysis provides computational efficiency by storing the eigensystem evaluations when

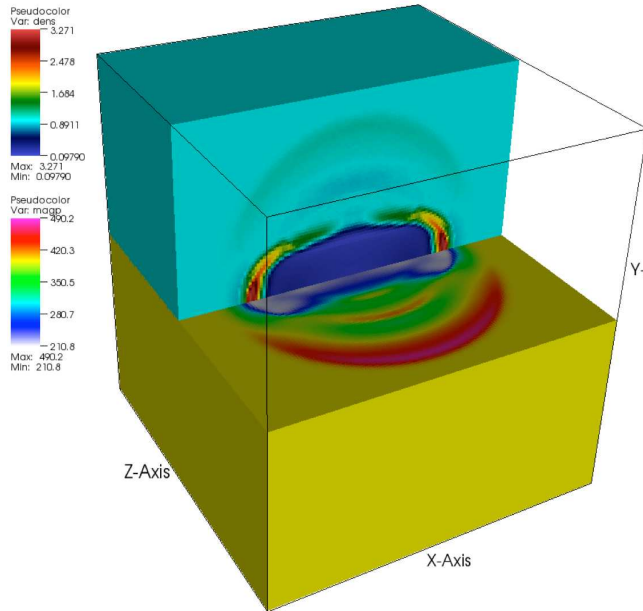


(a) Density and magnetic pressure at $t = 0.01$

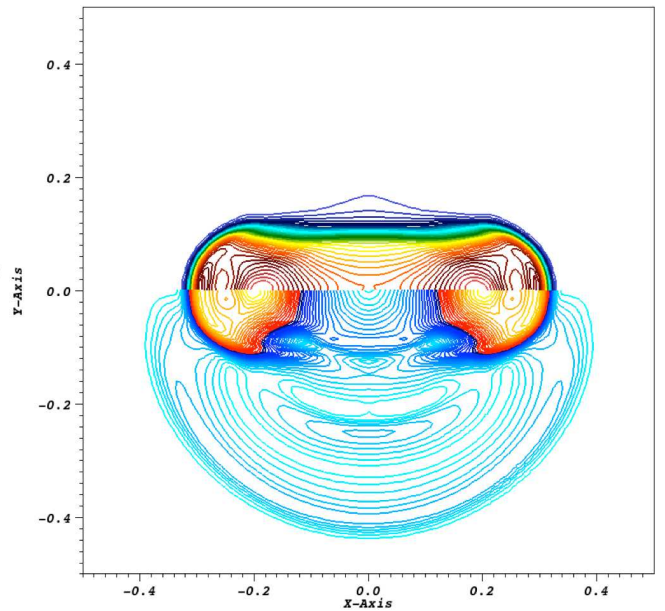


(b) Contours of gas pressure and total velocity at $t = 0.01$ in the $x-y$ plane at $z = 0$

Fig. 10. Results of the blast problem simulation with $B_x = \frac{50}{\sqrt{4\pi}}$ using a hybrid Riemann solver. In (a), density (denoted as "dens" in the legend) is plotted at the top half. Magnetic pressure (denoted as "magp" in the legend) is plotted at the bottom half. In (b), 40 contour lines are plotted for gas pressure (top half) between 0.009981 and 106.6 and total velocity (bottom half) between 0 and 11.84.



(a) Density and magnetic pressure at $t = 0.01$



(b) Contours of gas pressure and total velocity at $t = 0.01$ in the $x-y$ plane at $z = 0$

Fig. 11. Results of the blast problem simulation with $B_x = \frac{100}{\sqrt{4\pi}}$ using a hybrid Riemann solver. In (a), density (denoted as "dens" in the legend) is plotted at the top half. Magnetic pressure (denoted as "magp" in the legend) is plotted at the bottom half. In (b), 40 contour lines are plotted for gas pressure (top half) between 0.009161 and 202.9 and total velocity (bottom half) between 0 and 15.97.

computing each normal direction and re-using them in the transverse flux calculations.

We introduced two different methods, the reduced and full 3D CTU schemes. The reduced scheme can be considered as a straightforward extension of the 2D CTU algorithm of Colella [16], and is analogous to the 6-solve algorithm in 3D by Gardiner and Stone [31]. Although the reduced CTU scheme has a simple implementation for 3D, its stability limit is bounded by a CFL number less than 0.5. The full CTU scheme significantly improves this limited stability range and can utilize the maximum stability range of CFL number close to 1. This was achieved by taking into account the second- and third-order cross derivative terms in computing intermediate states at $n + \frac{1}{3}$ and $n + \frac{1}{2}$. Our full CTU scheme thus includes the multidimensional upwind information that is crucial to provide the full CFL limit. We also showed that the relative CPU cost of the full scheme compared to the reduced scheme is less than 1, indicating the cost efficiency of the full CTU scheme. The multidimensional MHD terms are also properly included in both normal and transverse directions.

Second, we extensively investigated the lack of numerical dissipation mechanisms in the existing CT algorithms, especially when there is a biased direction in advecting magnetic fields. In the small angle advection tests in 2D and 3D, we showed that the field loop simply can fail to be cleanly advected, and become distorted into non-circular or non-cylindrical shapes in most CT schemes. By contrast, the upwind-MEC scheme, by incorporating upwind information adds the needed numerical dissipation when taking the arithmetic average in CT. The algorithm enhances the previous MEC scheme [40] in that upwind-MEC maintains consistency of plane-parallel and grid-aligned flows [30].

The results of the test problems in Section 4 give considerable confidence in our scheme for use as a robust and reliable second-order, finite-volume 3D MHD algorithm. The methods developed in this paper for the 3D USM scheme preserve the divergence-free constraint without any evidence of numerical instability or accumulation of unphysical errors using a very high CFL number close to 1. The suite of test problems presented in this study include several stringent setups can be particularly challenging for MHD algorithms. The scheme has been thoroughly tested and has been shown to perform very well, providing confidence in its ability to correctly simulate a wide range of MHD phenomena.

The 3D USM scheme presented here has been implemented on both uniform and AMR grids. It has been integrated and tested in the official FLASH4 release of the Flash Center for Computational Science at the University of Chicago [29].

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